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(54) Title: MODIFIED DEACETOXYCEPHALOSPORIN C SYNTHASE (DAOCS) AND X-RAY STRUCTURE

#### (57) Abstract

Three-dimensional crystal structure(s) of deacetoxycephalosporin C synthase (DAOCS) are described. The X-ray co-ordinates provide precise 3-dimensional information of amino acids within the structure of DAOCS. Some of these are in complexes with iron and/or substrates. Information from the structures is used to modify enzymes of the cephalosporin biosynthesis pathway including DAOCS, deacetylcephalosporin C synthase DAOC/DACS, such that they accept unnatural substrates (e.g. penicillins G, V) in order to improve the production of beta-lactam antibiotics. The structures may be used to predict the structures of other 2-oxoglutarate dependent enzymes, thereby allowing the design of inhibitors, and new catalysts for the production of e.g. oxidised amino acids/peptides. Specific modifications of amino acid residues are proposed and exemplified.

> U.S. Patent Application No. 10/719,238 Attorney Docket No. 6653-021-999 Reference AN

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# MODIFIED DEACETOXYCEPHALOSPORIN C SYNTHASE (DAOCS) AND X-RAY STRUCTURE

- Penicillin and cephalosporin antibiotics are produced either directly by fermentation or by modification of fermentation derived materials containing a beta-lactam ring. The biosynthetic pathway to the penicillins and cephalosporins has been extensively studied and reviewed (J. E. Baldwin and C. J. Schofield, in 'The Chemistry of β-lactams (Ed. M. I. Page), Chapter 1, Blackie, London 1992; Ingolia and Queener, Med. Res. Rev., 1989, 9, 245-264; Aharonowitz, Cohen and Martin, Ann. Rev. Microbiol., 1992, 46, 461-495; Schofield, Bycroft, Baldwin, Hadju, Roach, Current Opinion in Structural Biology, 1997, 7, 857-864) and includes the following steps (Figure 1):
- Conversion of the tripeptide: <u>L</u>-δ-α-aminoadipoyl-<u>L</u>-cysteinyl-<u>D</u>-valine (ACV) to isopenicillin N in a step catalysed by isopenicillin N synthase (IPNS). This step is common to both penicillin and cephalosporin biosynthesis.
- In some organisms (e.g. Penicillium chrysogenum and Aspergillus nidulans) isopenicillin N is converted by exchange of its <u>L</u>-δ-α-aminoadipoyl side chain to penicillins with other side chains, which are normally more hydrophobic than the side chain of isopenicillin N. This conversion is catalysed by an amidohydrolase/ acyltransferase enzyme. Examples of penicillins produced by this biosynthetic process include penicillin G (which has a phenylacetyl side chain) and penicillin V (which has a phenoxyacetyl side chain). These hydrophobic penicillins may be commercially produced via fermentation under the appropriate conditions.
  - 3. In other organisms (e.g. *Streptomyces clavuligerus* and *Cephalosporium acremonium*) isopenicillin N is epimerised to penicillin N. This reaction is catalysed by an epimerase enzyme.

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- 4. In some organisms (e.g. S. clavuligerus and C. acremonium) penicillin N is converted to DAOC. This reaction is catalysed by deacetoxycephalosporin C synthase (DAOCS) in some organisms (e.g. Streptomyces clavuligerus) and by deacetoxy/deacety/cephalosporin C synthase (DAOC/DACS) in others (e.g. C. acremonium).
- 5. In some organisms (e.g. *S. clavuligerus* and *C. acremonium*) DAOC is converted to deacetylcephalosporin C (DAC). This reaction is catalysed by deacetylcephalosporin C synthase (DACS) in some organisms (e.g. *S. clavuligerus*) and by deacetoxy/deacetylcephalosporin C synthase (DAOC/DACS) in others (e.g. *C. acremonium*).

Further biosynthetic steps to give other cephalosporin derivatives may also occur, e.g. in *C. acremonium* DAC may be converted to cephalosporin C and in *Streptomyces spp.* DAC may be converted to cephamycin C. The genes encoding for each of the enzymes catalysing steps 1-6 above have been identified and sequenced.

Fermented penicillins, cephalosporins and their biosynthetic intermediates are useful as antibiotics or as intermediates in the production of antibiotics. Penicillins with hydrophobic side chains may be used for the preparation of cephalosporins or intermediates used in the preparation of cephalosporins, e.g. penicillins (including penicillin G and penicillin V) may be used to prepare C-3 exomethylene cephams which may be used as intermediates in the preparation of the commercial antibiotics, e.g. Cefachlor.

The enzymes IPNS, DAOCS, DACS and DAOC/DACS are

members of an extended family of Fe(II) utilising oxidase and oxygenase enzymes. Most of this family (including DAOCS, DACS and DAOC/DACS) utilise a 2-oxo acid (normally 2-oxoglutarate) as a cosubstrate in addition to dioxygen and the 'prime' substrate (e.g. penicillin N in the case of DAOCS). Since IPNS, does not use 2-oxoglutarate, it has a substantially different mechanism to the 2-oxoglutarate dependent oxygenases, and this gives

rise to a significantly different active site.

### The Invention

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This invention is based on the determination of the three dimensional crystal structure of DAOCS and the information and developments which come from it. The X-ray co-ordinates provide very detailed 3-dimensional information on the relationships between amino acid residues in the structure of DAOCS and on the binding modes of the Fe-cofactor and the substrates to DAOCS. The structure allows the modification of DAOCS and related enzymes of penicillin and cephalosporin biosynthesis (including DACS and DAOC/DACS) in order to alter their substrate and product selectivities. Since the DAOCS structures are the first from the family of 2-oxoglutarate dependent dioxygenases they also allow for the design of new inhibitors of this family of enzymes. Previously partial overviews of the structures of IPNS complexed to manganese and IPNS complexed to iron and ACV were reported (Roach et al., Nature, 1995, 375, 700-704; Roach et al., Nature, 1997, 387, 827). The structures, as defined by their X-ray co-ordinates, of IPNS complexed to manganese and in complexes with iron, ACV and/or substrate analogues have been reported in Baldwin, Hajdu, Roach, Hensgens, Clifton, GB 9621486.1- (Oxygenase Enzymes and Method).

Procedures have been developed for the production of 7-aminodeacetoxycephaosporin C (7-ADCA) in which recombinant *P. chrysogenum* strains into which the DAOCS gene has been introduced are used for the production of cephalosporins. In particular if adipic acid is added to these recombinant strains adipoyl-6-APA is produced, which is converted by DAOCS into adipoyl-7-ADCA from which the adipoyl side chain can be removed (EPA-A-0532341, Shibata *et al.*, Bioorg. Med. Chem. Letts, 1996, 6, 1579-1584).

The IPNS gene sequence (and therefore the amino acid

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sequence) is related but significantly different to those of DAOCS, DACS, DAOC/DACS. It is likely that gross elements of the fold (i.e. significant elements within the 3-dimensional structure) of these enzymes will be conserved but that the active site architecture will be very significantly different. Structural elements conserved are likely to include the betabarrel 'jelly roll' core and certain alpha-helices (including alpha helix-10, as defined in Roach et al., Nature, 1995, 375, 700-704). The degree of similarity is insufficient to define the precise structure of DAOCS, DACS, or DAOC/DACS from the IPNS structures. To date no models of DAOCS, DACS, or DAOC/DACS based on the IPNS structure have been reported. Nor have any detailed studies on substrate binding of these enzymes been reported. One report (WO 97/20053) claims the use of products resulting from modification of certain residues in DAOCS for the improved conversion of penicillin G to phenyl acetyl (G)-7-aminocephalosporanic acid.

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The three-dimensional structure of DAOCS is defined by the X-ray co-ordinates set out below (Structure A).

Also set out below is a high resolution crystal structure of a complex of prokaryotic DAOCS from *S. clavuligerus* with Fe(II) and 2-oxoglutarate (Structure B).

In part the present invention relates to the use of the structures of DAOCS in order to make modifications to it or DACS or DAOC/DACS in order that the modified enzymes catalyse the conversion of unnatural penicillins (e.g. penicillin G and penicillin V) to cephalosporins more efficiently than the wild-type enzyme. Further aspects of the invention relate to the use of the DAOCS structure in order to produce unnatural products in micro-organisms. Such products include exomethylene cephalosporins, with or without alpha-aminoadipoyl or hydrophobic side chain (e.g. phenylacetyl or phenoxyacetyl). Thus one aspect of this invention refers to the use of the structure of DAOCS for modifying DAOCS

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(or the closely related enzymes DACS or DAOC/DACS) in order to:

- permit the enzyme to accept (or accept more efficiently) unnatural penicillin substrates for the preparation of new or commercially valuable antibacterial materials.
- enable the modified enzyme to produce unnatural (e.g. (ii) exomethylene cephams) or optimise the production of minor products (e.g. 3- $\beta$ -hydroxycephams) for use as antibacterials or as intermediates in the preparation of antibacterials or commercially valuable compounds.

In another aspect this invention provides modified enzymes that result from application of the aforementioned techniques. These are 10 enzymes having significant (as defined below) sequence and thus structural similarity with DAOCS. Thus, structures of these enzymes may be predicted on the basis of the DAOCS structures. Preferably there will be sequence similarity/identity between most of the modified enzyme and a major part of DAOCS. Previous sequence comparisons (Roach et al., 15 Nature, 1995, 375, 700), using pairwise comparisons of the sequences followed by single linkage cluster analysis show that IPNS, DAOCS, DACS and DAOC/DACS cluster with standard deviations scores of >5.0 (Barton and Sternberg, J. Mol. Biol., 1987, 198, 327). Scores over 5.0 and preferably over 6.0 indicate that the sequence alignments will be correct 20 within all or most of the protein secondary structural elements (Barton, Methods in Enzymol., 1990, 183, 403); thus they have significantly similar sequences and hence structures. Note there are other criteria which may be used to ascertain significant sequence similarity for example % identity or % similarity of amino acids possessing side chains with similar physicochemical properties (Barton and Sternberg, J. Mol. Biol., 1987, 198, 327). Thus, on the basis of sequence comparisons it is possible to predict the structure of one enzyme (e.g. DACS or DAOC/DACS) from another closely related enzyme (e.g. DAOCS). Further, it is recognised that although two enzymes may have structures in which secondary structural elements are

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largely or wholly conserved, differences in the structures of the two enzymes may result from the side chains of the amino acids forming the secondary structural elements. The effect of these differences, which alter the substrate/product selectivities of the compared enzymes, is predictable once the three-dimensional structure of one of the enzymes is known.

In another aspect the invention provides an enzyme having significant (as herein define 1) sequence similarity to DAOCS wherein the side chain binding site of penicillin N or DAOC is modified and at at least one of the following sites at least one amino acid residue is changed to another amino acid residue or is deleted: Thr72, Arg74, Arg75, Glu156, Leu158, Arg160, Arg162, Leu186, Ser187, Phe225, Phe264, Arg266, Asp301, Tyr302, Val303, Asn304; and/or at least one additional amino acid residue is inserted within the region 300-311; provided that other residues interacting with the above may be changed in order to accommodate the change in one of the above.

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Modifications of this kind will permit the expansion of penicillin V or penicillin G to the corresponding cephalosporins. To achieve this it is desirable to increase the kcat/Km for the mutant as compared to the wild type DAOCS. Kinetic results indicate that apparent kcat values for penicillin N and penicillin G are similar but that Km is much higher for penicillin G. Thus based on these analysis, a decrease in the binding constant of DAOCS for penicillin G should make it possible to increase kcat/Km for penicillin G.

The side chain binding pocket of DAOCS is made of residues from different parts of the peptide chain, so it is likely that more than one residue will have to be altered to make a better penicillin G/V expander. Nevertheless some residues are more important than others. Examination of the interactions between the last few C-terminal residues (Thr-308 to Ala-311) of one DAOCS molecule and the active site of another in the crystal structure, suggests a binding mode for the penicillin nucleus which

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is shown in Figure 2 of the accompanying drawings. The penam C-3 carboxylate group probably occupies an analogous position to that of Ala-311 from a symmetry related molecule in the active site, forming electrostatic interactions with Arg-162 and Arg-160. The side chain of Arg-160 may also form a hydrogen bonding interaction with the  $\beta$ -lactam carbonyl.

It needs to be borne in mind that protein specificity is generally controlled by more than one amino acid. To alter the specificity of a protein in a major way is likely to require more than one of the mutational changes suggested below, although each of the mutations will contribute. With this in mind, preferred residues to modify for the expansion of a penicillin are as follows:

- a) Arg-266. This residue binds with the  $\alpha$ -aminoadipate side chain of the natural substrate and should be changed to a residue of more hydrophobic character, e.g. Phe, Ala, Val, Leu, Ile.
- b) Thr-72. This should be changed to a hydrophobic residue e.g. Val, Leu, Ile, Phe, Ala, to help bind the hydrophobic side chain of penicillin G. It should be effective in combination with other mutants.
- c) Arg-74 may be usefully changed to a neutral or hydrophobic residue (Phe, Tyr, Val, Leu, Ile, Ala). Modification of Arg-75 may be necessary in addition because it forms a hydrogen-bonding network with-Arg-74.
- d) Glu-156. This residue binds with the  $\alpha$ -aminoadipate side chain. It should be changed to one of Ala, Val, Leu, Ile, Phe, Tyr, Trp, Asn, Gln, Ser.
- e) The side chains of Leu-158, Asn-301 and Tyr-302 form part of the binding pocket for the penicillin side chain and can be usefully modified to more hydrophobic character.
  - f) Asn-304. This residue binds the amide linking the side chain to the penam nucleus. Modification is effected to expand penicillins with shortened or no side chains (e.g. to Asp or Glu for 6-Apa).

Note that other changes may be used to construct part or all of a side chain binding pocket via hydrogen bonding or other interactions.

The insertion or deletion of residues into the DAOCS sequence may also be of use in constructing a hydrophobic binding pocket for the penicillin side chain. Insertion of hydrophobic residues into the C-terminal region (residue 300-311 and in particular 301-303) may assist in the construction of a hydrophobic binding pocket for penicillin side chains.

In another aspect the invention provides an enzyme having significant (as herein defined) sequence similarity to DAOCS wherein the penicillin/cephalosporin binding site of penicillin N or DAOC is modified and at at least one of the following amino acid residues is changed or deleted: Ile88, Arg160, Arg162, Phe164, Met180, Thr190, Ile192, Phe225, Pro241, Val245, Val262, Phe264, Asn304, Ile305, Arg306, Arg307; and/or at least one additional amino acid residue is inserted within the region 300-311; provided that other residues interacting with the above may be changed in order to accommodate the change in one of the above.

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Further discussion of this aspect may be found in Nature Volume 394, pages 805-809 published on 20 August 1998 and incorporated by reference herein.

Another aspect of the invention refers to the use of the structure of DAOCS in order to modify its active site (or that of a structurally related 2-oxoglutarate dependent dioxygenase) in order that the modified enzyme accepts non beta lactam substrates in order to produce oxidised compounds of value. Oxidised amino acids (e.g. 4-hydroxyprolines, hydroxylysines, hydroxyaspartic acids and others) are useful as synthetic intermediates in the production of valuable materials. Using the structure of DAOCS specific residues can be targeted for modification in order that the modified enzyme can be used to produce oxidised amino acids or peptides. The process may include modification of the following residues:

Arg74, Glu156, Leu158, Arg160, Arg162, Leu186, Ser187, Phe225, Phe264, Arg266, Asp301, Tyr302, Val303, Asn304, Ile88, Arg162, Phe164, Met180, Thr190, Ile192, Pro241, Val245, Val262, Ile305, Arg306, Arg307.

DAOCS structure for the design of selective inhibitors of 2-oxoglutarate dependent dioxygenases. The 2-oxoglutarate dependent dioxygenase prolyl 4-hydroxylase has been the target of inhibition in order to provide a therapeutic treatment for fibrotic diseases (e.g. liver cirrhosis, arthritis).

However, no inhibitors are in clinical use, probably because it is difficult to achieve selective inhibition of the target enzyme for inhibition over other enzymes (including 2-oxoglutarate dependent enzymes). The structure of DAOCS provides a template for the design of inhibitors of 2-oxoglutarate dependent dioxygenases.

Set out below are two high resolution crystal structures for DAOCS from *S. clavuligerus:* the structure of the iron-free apoenzyme (Structure A) and the structure of the complex with Fe(II) and 2-oxoglutarate (Structure B). The results imply a mechanism by which the enzyme-Fe(II) complex reacts with 2-oxoglutarate and dioxygen to give the reactive ferryl species, a process common to many non-haem oxygenases. Other notable 2-oxoacid-dependent ferrous enzymes are prolyl hydroxylase, involved in collagen biosynthesis, gibberellin 3β-hydroxylase, a mutation of which influences stem length in plants, and clavaminic acid synthase, involved in the biosynthesis of the β-lactamase inhibitor, clavulanic acid. Within the family of 2-oxoacid-dependent enzymes, DAOCS belongs to a sub-family, the members of which show sequence similarity with IPNS and 1-aminocyclopropane-1-carboxylate oxidase (the ethylene forming enzyme), enzymes that do not use a 2-oxoacid in catalysis.

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as a crystallographic trimer. The main chain of the protein folds into a conserved jelly roll core with flanking helices.

Co-ordinates and structure factors have been deposited with the Protein Data Bank (entries 1rxg, and r1rxgsf for the Fe(II)-2-oxoglutarate complex).

### LEGENDS TO FIGURES.

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Figure 1: the biosynthetic pathway to the penicillins and cephalosporins.

Figure 2 is a view of the active site of DAOCS showing 2-oxoglutarate binding to the iron and proposed penicillin N binding. Interactions with the side chains of certain amino acid residues are indicated by arrows.

Structure A is a three-dimensional structure of DAOCS.

Structure B is a high resolution crystal structure for prokaryotic DAOCS from *S. clavuligerus* as a complex with Fe(II) and 2-oxoglutarate.

The peptide sequence of DAOCS (with the numbering used herein) is set out below:

	Met	Asp	Thr	Thr	Val	Pro	Thr	Phe	Ser	Leu	10
	Ala	Glu	Leu	Gln	Gln	Gly	Leu	His	Gln	Asp	20
	Glu	Phe	Arg	Arg	Cys	Leu	Arg	Asp	Lys	Gly	30
	Leu	Phe	Tyr	Leu	Thr	Asp	Cys	Gly	Leu	Thr	40
5	Asp	Thr	Glu	Leu	Lys	Ser	Ala	Lys	Asp	Leu	50
	Val	Ile	Asp	Phe	Phe	Glu	His	Gly	Ser	Glu	60
	Ala	Glu	Lys	Arg	Ala	Val	Thr	Ser	Pro	Val	 70
	Pro	Thr	Met	Arg	Arg	Gly	Phe	Thr	Gly	Leu	80
	Glu	Ser	Glu	Ser	Thr	Ala	Gln	Ile	Thr	Asn	90
10	Thr	Gly	Ser	Tyr	Ser	Asp	Tyr	Ser	Met	Cys	100
	Tyr	Ser	Met	Gly	Thr	Ala	qzA	Asn	Leu	Phe	110
	Pro	Ser	Gly	Asp	Phe	Gly	Arg	Ile	Trp	Thr	120
	Gln	Tyr	Phe	qzA	Arg	Gln	Tyr	Thr	Ala	Ser	130
	Arg	Ala	Val	Ala	Arg	Glu	Val	Leu	Arg	Ala	140
15	Thr	Gly	Thr	Glu	Pro	Asp	Gly	Gly	Val	Glu	150
	Ala	Phe	Leu	Asp	Cys	Glu	Pro	Leu	Leu	Arg	160
	Phe	Arg	Tyr	Phe	Pro	Gln	Val	Pro	Glu	His	170
	Arg	Ser	Ala	Glu	Glu	Gln	Pro	Leu	Arg	Met	180
	Ala	Pro	His	Tyr	qaA	Leu	Ser	Met	Val	Thr	190
20	Leu	Ile	Gln	Gln	Thr	Pro	Cys	Ala	Asn	Gly	200
	Phe	Val	Ser	Leu	Gl'n	Ala	Glu	Val	Gly	Gly	210
	Ala	Phe	Thr	qzA	Leu	Pro	Tyr	Arg	Pro	Asp	220
	Ala	Val	Leu	Val	Phe	Cys	Gly	Ala	Ile	Ala	230
	Thr	Leu	Val	Thr	Gly	Gly	Gln	Val	Lys	Ala	240
25	Pro	Arg	His	His	Val	Ala	Ala	Pro	Arg	Arg	250
	Asp	Gln	Ile	Ala	Gly	Ser	Ser	Arg	Thr	Ser	260
	Ser	Val	Phe	Phe	Leu	Arg	Pro	Asn	Ala	Asp	270
	Phe	Thr	Phe	Ser	Val	Pro	Leu	Ala	Arg	Glu	280
	Cys	Gly	Phe	Asp	Val	Ser	Leu	Asp	Gly	Glu	290
30	Thr	Ala	Thr	Phe	Gln	Asp	Trp	Ile	Gly	Gly	300
	Asn	Tyr	Val	Asn	Ile	Arg	Arg	Thr	Ser	Lys	310
	Ala										311

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# STRUCTURE A

CRYST1	106.400	106.400	) 7	1.100	90.00	90.00	120.00
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SCALE3	0.000	0000	0.000000	0.0140	065	0.0000	00

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 ANISOU 3
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N AASP 2
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CB AASP 2
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 MOTA
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 ANISOU 15
 ATOM
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 ANISOU 16
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ATOM 17 N
ANISOU 17 N
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31.874 13.050 57.425 0.458 40.62
                                                                    -105 1580 477
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ATOM 18 CA BMET 1 31.874 13.050 57.425 0.458 40.62
ANISOU 18 CA BMET 1 4228 4809 6395 580 210 16
ATOM 19 C BMET 1 30.884 14.113 57.894 0.458 38.21
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ANISOU 21 CB BMET 1 4866 2613 5114 2013 -122 81
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ANISOU 24 CE BMET 1 10672 4519 5420 1149 4083 -2
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BASP ^
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ANISOU 25 N
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ANISOU 26 CA BASP 2
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ANISOU 27 C BASP 2
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28:181 14.602 58.414 0.732 34.65
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ANISOU 28 O BASP 2
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CB BASP 2
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MOTA
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ATOM	40	N	THR	4	26.036	16.780	60.456		32.55
ANISOU	40	N	THR	4	4306	4611	3450	377	-2166 -217
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ANISOU ATOM	41 42	CA	THR	4	4275	4229	3358	-81	-1179 9 5
ANISOU	42	C	THR THR	4	24.672	18.272	59.090		30.06
ATOM	43	0	THR	4 4	4876 25.195	3341 17.935	3207 58.017	773	-1156 - 204
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ATOM	46		THR	4	25.852	20.582		1.000	27.22
ANISOU	46		THR	4	3728	4174	2443		4 - 1 5 1
ATOM	47	N	VAL	5	23.464	18.796	59.211		
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ATOM ANISOU	48 48	CA	VAL	5	22.690	19.140	58.024		
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ANISOU	49	C	VAL	5	23.199 2263	20.489 1803	57.499 2396	-279	-622 8 9
ATOM	50	Ô	VAL	5	23:156	21.449	58.252		
ANISOU	50	Ö	VAL	5	3662	1885	2472	-389	-656 1 6
ATOM	51	СВ	VAL	5	21.204	19.216	58.402		
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ATOM	53		VAL	5	20.701	17.867			28.58
ANISOU ATOM	53 54		VAL	5	5258	2086	3516	-1226	
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ATOM	55	CA	PRO PRO	6	2378	1629	2434	29 -5	
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ATOM	56	C	PRO	6	23.298	22.800	55 323		15.61
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AŤŐM	57	Ö	PRO	6	22.133	22.432	55.201		
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ATOM	58	СВ	PRO	6	25.216	21.375			19.85
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ATOM	60	CD	PRO	6	23.926	19.428			17.91
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ATOM ANISOU	61 61	N	THR	7	23.723	24.031			14.38
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                                2619
                                        3175 -183 -732 -408
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- 17 -NE2 GLN 14 18.398 30.513 41.349 1.000 23.60 ATOM 123 ANISOU 123 NE2 GLN 14 3058 2941 2969 -383 54 2 4 5 M GLN 15 25.309 31.243 41.395 1.000 25.00 ANISOU 124 GLN 15 3078 3281 3140 -1159 -394 5 7 5 ATOM 125 CA GLN 15 26.530 31.936 40.945 1.000 24.05 ANISOU 125 CA GLN 15 2947 3560 2631 -866 -98 655 ATOM 126 27.650 30.920 С GLN 15 40.707 1.000 26.06 ANISOU 126 С GLN 15 3810 3951 2139 -345 406 668 ATOM 127 0 GLN 15 28.756 31.284 40.302 1.000 35.85 15 ANISOU 127 0 GLN4294 4851 4476 102 1871 1192 15 ATOM 128 CB GLN 27.018 32.918 42.009 1.000 25.90 15 15 15 ANISOU 128 3055 3037 26.103 34.092 CB GLN 3748 -1092 -109 3 6 4 ATOM 129 CG GLN 42.219 1.000 31.24 4562 2577 26.503 35.022 9927 2477 ANISOU 129 CG GLN15 4731 -806 962 1054 ATOM 130 CD GLN 15 43.348 1.000 59.75 15 ANISOU 130 CD GLN 10301 -1855 -14 -1904 27.634 35.031 43.840 1.000 81.81 OE1 GLN 15 ATOM 131 OE1 GLN 15 ANISOU 131 15059 12094 -944 -6272 -1803 43.767 1.000 91.46 3931 ATOM NE2 GLN 15 25.539 35.841 132 ANISOU 132 NE2 GLN 15 14070 15833 -923 3672 -4850 40.969 1.000 29.90 4846 ATOM 133 N 27.379 29.643 GLY 16 ANISOU 133 N GLY16 4634 3820 2907 -239 22 7 8 7 MOTA 134 CA GLY 16 28.410 28.649 40.699 1.000 28.76 16 4466 ANISOU 134 CA GLY 3629 2833 -709 461 250 MOTA 16 29.339 28.473 41.878 1.000 27.60 135 С GLY 16 ANISOU 135 С GLY 3816 3779 2891 -616 914 1485 16 ATOM 136 0 GLY30.398 27.867 41.725 1.000 31.47 ANISOU 136 O GLY 16 3386 4758 3814 16 3386 4758 3814 -899 1243 1 17 28.960 28.898 43.083 1.000 26.01 -899 1243 1023 ATOM 137 N LEU 17 ANISOU 137 N LEU 3295 3636 2950 -721 162 743 138 CA LEU 17 29.776 28.666 44.257 1.000 23.96 ANISOU 138 CA LEU 17 2700 3032 3372 -601 100 673 ATOM 139 C 29.462 27.338 44.932 1.000 20.31 LEU 17 ANISOU 139 C LEU 17 2222 2763 2733 -252 611 ATOM 140 O LEU 17 28.389 26.780 44.789 1.000 23.13 ANISOU 140 O LEU 17 2347 3308 3134 263 859 -443 ATOM 141 CB LEU 17 29.645 29.806 45.286 1.000 25.94 ANISOU 141 17 CB LEU 2886 2933 4035 -1318 -405 2 5 4 CG LEU CG LEU CD1 LEU ATOM 142 17 29.962 31.209 44.716 1.000 31.57 ANISOU 142 17 3741 2948 5308 -523 1150 7 2 2 ATOM 17 143 29.550 32.358 45.615 1.000 32.04 ANISOU 143 CD1 LEU 17 5221 2887 4066 -1269 278 5 0 8 31.458 31.278 44.416 1.000 38.11 ATOM 144 CD2 LEU 17 CD2 LEU 17 ANISOU 144 3828 5491 5160 -2315 954 2 3 2 30.441 26.822 45.681 1.000 22.49 145 N MOTA 18 HIS ANISOU 145 N 18 HIS 2600 3067 2877 -662 42 4 4 9 ATOM 30.289 25.644 46.537 1.000 21.54 146 CA HIS 18 ANISOU 146 CA HIS 18 2378 2809 2996 -432 201 313 ATOM 147 C HIS 18 29.908 24.376 45.790 1.000 22.76 ANISOU 147 C HIS 18 2256 3245 3148 -1009 282 114 ATOM 148 0 HIS 18 29.147 23.565 46.331 1.000 22.60 ANISOU 148 O HIS 18 2008 3064 3516 -629 -166 8 8 4 MOTA 149 CB HIS 18 29.224 25.872 47.618 1.000 22.81 ANISOU 149 СВ HIS 18 2514 2879 3272 -526 450 421 ATOM 150 CG 18 HIS 29.320 27.248 48.217 1.000 21.70 ANISOU 150 CG HIS ND1 HIS CG 18 2797 3038 2411 -149 39 5 0 3 MOTA 151 18 30.438 27.773 48.807 1.000 25.01 ANISOU 151 ND1 HIS 18 3714 3505 2234 -207 -629 1 4 9 152 ATOM CD2 HIS 18 28.370 28.216 48.269 1.000 24.95 ANISOU 152 CD2 HIS 18 3244 3278 2957 87 544 2 7 5 MOTA 153 CE1 HIS 18 30.197 28.982 49.223 1.000 29.26

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- 18 -
 ANISOU 153
            CE1 HIS 18 4603
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                                         3118
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        154
             NE2 HIS 18 28.937 29.271 48.919 1.000 27.24
            NE2 HIS 18
 ANISOU 154
                         4582
                                 3137
                                         2632
                                                2 224 365
 MOTA
        155
             Ν
                GLN
                     19
                         30.269
                                 24.270 44.521 1.000 22.74
ANISOU 155
             N
                GLN
                     19
                         2724
                                 3094
                                         2822
                                                -511 -123 4 2 3
 ATOM
        156
                     19
            CA GLN
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ANISOU 156
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                         3129
                                 2668
                                         3263
                                                148
                                                      63 8 9
MOTA
        157
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                     19
                         30.271
                                 21.760 44.221 1.000 22.77
ANISOU 157
            С
                     19
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                         2532
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                                         3095
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ATOM.
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ANISOU 158
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                GLN
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                         1869
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ATOM
       159
            CB GLN
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                                 23.322
ANISOU 159
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                     19
                         5043
                                 2519
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ATOM
       160
            CG GLN
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ANISOU 160
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                GLN
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                                                299
                                                      171 4 3 7
ATOM
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ANISOU 161
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                                                -986
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ATOM
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ATOM
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ATOM
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ANISOU 164
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                ASP
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                                        3123
                                                -414 95 7 0 8
ATOM
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            CA ASP
                         31.926 20.292 45.225 1.000 23.10
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ANISOU 165 CA ASP
ATOM 166 C ASP
ANISOU 166 C ASP
ATOM 167 O ASP
-ANISOU 167 O ASP
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                         1775
                                         2873 -280 -143 4 9 3
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20 1429
                                 18.899 46.768 1.000 21.48
                                 2884 3848 -311 225 2 2 4
20.268 45.521 1.000 27.66
ATOM 168 CB ASP
ANISOU 168 CB ASP
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                     20
                         1835
                                 4546
                                         4130
                                                -16
                                                      207 881
ATOM
       169 CG ASP
                     20
                         34.298
                                 20.206 44.291 1.000 39.35
ANISOU 169 CG ASP
                     20
                         2355
                                 6893
                                         5705
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ATOM
       170
            OD1 ASP
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                     20
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            OD1 ASP
ANISOU 170
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MOTA
       171
            OD2 ASP
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                         35.508 20.433 44.467 1.000 45.22
ANISOU 171
            OD2 ASP
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                                                -589 1088 - 87
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MOTA
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                GLU
                     21
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ANISOU 172
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                GLU
                     21
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                                         3093
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                                                     -241 3 6 7
ATOM
       173
            CA GLU
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                         30.323
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ANISOU 173 CA GLU
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                                 2956
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                                                -481 -464 1 1 8
      174 C
MOTA
                GLU
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                                        48.402 1.000 17.84
ANISOU 174 C
                GLU
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ATOM
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                GLU
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ANISOU 175 O
                GLU
                     21
                         1671
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                                         3057
                                                -419
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ATOM 176
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ATOM 177
ANISOU 177
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            СG
                GLU
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                                                -766
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                                         3912
                                                     -326 - 711
ATOM
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                                                -752 -666 5 2 1
ATOM
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                                 23.594 47.887 1.000 35.14
ANISOU 179
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                                 4054
                                        6677 -1336 -1741 1977
ATOM
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ANISOU 180
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ATOM
       181
            \mathbf{N}
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                PHE
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MOTA
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ANISOU 182
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MOTA
        183
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                PHE
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ANISOU 183
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ANISOU 192 N ARG 23
ATOM 193 CA ARG 23
ANISOU 193 CA ARG 23
ATOM 194 C ARG 23
ANISOU 194 C ARG 23
ATOM 195 O ARG 23
ANISOU 195 O ARG 23
ANISOU 196 CB ARG 23
ANISOU 196 CB ARG 23
ANISOU 196 CB ARG 23 1647 2437 2709 -168 -218 3 1 7 27.520 17.594 45.079 1.000 19.18 1724 2539 3022 -166 36 1 5 8 27.767 16.595 46.211 1.000 19.11 1279 2461 3518 -173 -113 4 5 5 27.107 15.547 46.229 1.000 18.82 1614 2156 3381 -33 181 -1 28.605 17.351 44.030 1.000 22.81 181 - 128 ANISOU 196 CB ARG 23 1934 4099 2633 -34 -105 -1 28.248 17.790 42.617 1.000 24.82 1934 -105 - 354ATOM 197 CG ARG ANISOU 197 CG ARG 23 23 2601 4078 2752 191 -122 - 204ATOM 198 CD ARG ANISOU 198 CD ARG 29.376 17.272 41.685 1.000 29.71 23 23 2503 5619 3168 -285 908 704 MOTA NE NE 199 ARG 23 18.206 41.800 1.000 30.96 30.479 ANISOU 199 ARG 23 2877 3851 -43 5034 286 ATOM 200 CZARG 23 30.549 19.360 41.148 1.000 ?9.49 ANISOU 200 CZ ARG 23 2612 5063 3529 ~-225 606 201 NH1 ARG 23 29.536 19.665 40.328 1.000 29.26 ANISOU 201 NH1 ARG 23 3242 4951 2923 -960 331 525 ATOM 202 NH2 ARG 23 31.629 20.092 41.345 1.000 32.61 ANISOU 202 NH2 ARG 23 2320 23 2320 5347 4722 -134 519 179 24 28.708 16.851 47.125 1.000 17.80 ATOM 203 N ARG ANISOU 203 N ARG 24 1262 2168 3332 183 38 9 8
ATOM 204 CA ARG 24 28.930 15.899 48.222 1.000 18.85
ATOM 205 C ARG 24 1368 2509 3287 69 -162 105
ANISOU 205 C ARG 24 27.701 15.811 49.114 1.000 17.51
ATOM 206 C ARG 24 1456 2015 3181 132 -177 2
ANISOU 206 C ARG 24 27.333 14.733 49.544 1.000 17.93
ANISOU 206 C ARG 24 1851 1965 2997 -16 -402 2
ANISOU 207 CB ARG 24 30.203 16.321 48.991 1.000 19.88
ATOM 208 CG ARG 24 1685 2700 3169 -398 -218 4 ANISOU 203 N ARG 1368 2509 3287 69 -162 105 27.701 15.811 49.114 1.000 17.51 3181 13.2 -177 2 4 3 -402 2 5 3 3169 -398 -218 4 4 208 CG ARG MOTA 31.459 16.053 48.135 1.000 29.07 24 ANISOU 208 CG ARG 24 1467 4625 4954 269 203 709 ATOM 209 CD ARG 32.700 16.206 49.016 1.000 41.84 24 ANISOU 209 CD ARG 24 1745 7021 7130 -451 -494 - 922 ATOM 210 NE ARG 24 33.690 17.103 48.464 1.000 57.06 ANISOU 210 NE ARG 24 8003 4362 9316 -3326 -669 -1141 ATOM 211 CZARG 24 34.032 18.327 48.810 1.000 60.67 ANISOU 211 CZ ARG 24 5961 10369 6723 -4627 -1324 -1586 ATOM 212 18.980 49.799 1.000 49.70 NH1 ARG 33.430 24 ANISOU 212 NH1 ARG 24 7748 6565. 4569 -951 -2185 2226 MOTA 213 NH2 ARG 34.997 24 18.971 48.159 1.000 54.12 ANISOU 213 NH2 ARG 24 8696 8490 3378 -3780 -2352 1607 214 N ATOM CYS 25 27.092 16.963 49.370 1.000 15.74

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ATOM ANISOU ATOM	21556677889900112223344556677888990011222333334455667788899	CD12 CD22 N CA CC C O O CB N CA N CA CC C O O CB D C C C O O C C C C C O O C C C C C O O C	ASP	22222222222222222222222222222222222222	143.88 2 4 1 7 0 3 1 4 1 5 1 4 1 5 1 4 1 4 1 5 1 4 1 4 1 5 1 4 1 5 1 4 1 5 1 4 1 5 1 4 1 5 1 4 1 5 1 4 1 5 1 4 1 5 1 4 1 5 1 4 1 5 1 4 1 5 1 4 1 5 1 6 1 6 1 7 7 8 1 1 2 1 6 1 5 1 7 2 1 6 1 5 1 7 2 1 6 1 5 1 7 2 1 6 1 5 1 7 2 1 6 1 5 1 7 2 1 6 1 5 1 7 2 1 6 1 5 1 7 2 1 6 1 6 1 8 1 7 1 7 1 7 1 7 1 7 1 7 1 7 1 7 1 7	96.94 68 2 196.94 68 2 180.36 16.99 26 2 180.36 17.86 18.39 8 151.37 16.43 15.39 8 171.64 15.39 8 171.64 15.39 8 171.66	2646.33	-95
ATOM ANISOU ATOM ANISOU	237 237 238 238	CB CB CG CG	ASP ASP ASP ASP	28 28 28 28	27.306 1581 28.590 1596	12.237 3894 11.906 3323	51.657 2948 50.941 4472	1.000 22.17 -272 -467 5 5 9 1.000 24.72 236 -288 6 4 8
ANISOU ATOM ANISOU ATOM ANISOU ATOM ANISOU ATOM ANISOU	239 240 241 241 242 242 243 243		ASP ASP		28.572	10.905	50.199 5084 51.251 6261 51.821 2627 52.778 2165 52.118 2686	1.000 27.56

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            C
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                         1479
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ATOM
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                TYR
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ANISOU 276
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ATOM
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MOTA
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ATOM
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2478 1967
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57.799 1.000 19.58
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ATOM
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ATOM
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ANISOU 281
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ATOM
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ANISOU 282
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ATOM
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ANISOU 283
            CZ
                TYR
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ATOM
       284
            \mathsf{OH}
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ANISOU 284
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                TYR
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ATOM
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                LEU
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ANISOU 285
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                LEU
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ATOM
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                LEU
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ANISOU 286
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ATOM
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ANISOU 287
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ATOM
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ATOM
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ATOM
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MOTA
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ANISOU 291
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ATOM
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ANISOU 292
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ATOM
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                THR
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ANISOU 293
           Ν
                THR
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ATOM
       294
           CA THR
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ANISOU 295
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ATOM
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ATOM
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ANISOU 297
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ATOM
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           OG1 THR
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ATOM
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ANISOU 299
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ATOM
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- 23 -MOTA 306 OD1 ASP 36 20.061 34.886 51.457 1.000 26.16 ANISOU 306 OD1 ASP 36 2981 2100 4860 378 -777 - 381 ATOM 307 OD2 ASP 36 21.824 33.982 50.528 1.000 24.87 ANISOU 307 OD2 ASP 36 2532 1994 4924 -49 -950 -628 308 ATOM И CYS 37 16.282 32.196 48.971 1.000 20.25 ANISOU 308 CYS Ν 3 7 2135 1711 3849 118 -638 - 263 ATOM 309 CA CYS 37 15.463 31.587 47.902 1.000 20.28 ANISOU 309 CACYS 37 2390 1478 3839 -799 - 138 136 ATOM 310 C CYS 37 14.078 32.183 47.818 1.000 19.90 CYS ANISOU 310 C 37 2374 1724 3463 214 -711 - 74 ATOM 311 0 CYS 37 13.176 31.629 47.156 1.000 22.75 ANISOU 311 0 CYS 37 2569 1984 4091 -12 -1108 1 5 ATOM 312 CB CYS 37 15.359 30.061 48.083 1.000 22.21 ANISOU 312 CВ CYS 37 2739 1454 4247 194 -477 - 115ATOM 313 SG CYS 37 14.500 29.595 49.596 1.000 22.84 ANISOU 313 37 SG CYS 2854 1884 3942 -203 -922 1 4 1 13.855 33.390 48.314 ..000 20.85 ATOM 314 N GLY38 ANISOU 314 N GLY 38 2353 1538 3933 217 -375 - 42ATOM CA GLY 315 38 12.570 34.044 48.194 1.000 23.42 ANISOU 315 CA GLY 38 2233 1874 4790 255 -292 1 6 5 ATOM C 316 GLY38 11.534 33.619 49.217 1.000 23.29 ANISOU 316 C GLY 38 2577 2045 4228 113 -136 -601 10.400 34.091 49.129 1.000 25.58 MOTA 317 0  $\operatorname{\mathsf{GL}} \operatorname{Y}$ 38 ANISOU 317 O  ${ t GLY}$ 38 2529 3424 3765 214 -96 -264 39 11.894 32.836 50.237 1.000 24.55 ATOM 318 N LEU ANISOU 318 N LEU 39 2310 2980 4037 119 -46 -364 319 CA LEU ATOM 39 10.938 32.331 51.195 1.000 24.44 ANISOU 319 CA LEU LEU 39 2637 2964 3684 -105 175 -1 LEU 39 11.107 32.885 52.593 1.000 35.41 3684 \_\_ -105 175 -946 MOTA 320 C ANISOU 320 C 39 5341 LEU 4215 3898 -796 165 -1435 3 9 3 9 MOTA 321 0 LEU 11.784 32.313 53.441 1.000 43.41 ANISOU 321 0 LEU 7338 4986  $4171 \sim -2639 - 1333 - 303$ CB LEU ATOM 322 39 10.850 30.810 51.206 1.000 26.48 ANISOU 322 CB LEU 39 4244 2879 2940 49 -70 - 261 ATOM 323 CG LEU 39 10.404 30.097 49.921 1.000 30.21 ANISOU 323 CG LEU 39 4834 2452. 4195 258 -1618 -474 ATOM 324 CD1 LEU 39 10.683 28.595 49.972 1.000 24.78 ANISOU 324 CD1 LEU 39 3351 2597 3468 424 -707 - 118ATOM 325 CD2 LEU 39 30.407 49.640 1.000 27.50 8.940 ANISOU 325 CD2 LEU 39 4828 2118 3503 860 -860 - 323ATOM 326 N THR 40 10.365 33.957 52.882 1.000 45.58 ANISOU 326 N THR 40 4849 7392 5077 -520 2852 -1993 ATOM CA THR 40 327 10.610 34.661 54.136 1.000 32.50 ANISOU 327 CA THR 40 4224 3732 4393 999 961 - 558 ATOM 328 C THR 40 9.700 34.177 55.248 1.000 29.68 ANISOU 328 С THR 40 3175 4204 3898 -116 294 -1630 ATOM 329 0 THR 40 8.653 33.556 55.031 1.000 39.75 ANISOU 329 THR 0 40 3930 5847 5326 -1079 -301 -1653 ATOM 330 CB THR 10.641 36.183 53.997 1.000 56.31 40 CB THR ANISOU 330 40 10586 3758 7052 -1417 1006 - 992 11.545 36.606 52.946 1.000 68.39 OG1 THR MOTA 331 40 ANISOU 331 OG1 THR 7379 40 3900 14707 -1978 3617 - 246 ATOM 332 CG2 THR 11.214 36.837 55.256 1.000 70.22 40 ANISOU 332 CG2 THR 40 8265 5228 13188 1389 -4422 -3241 MOTA 333 N ASP 41 10.191 34.302 56.486 1.000 33.20 ANISOU 333 ASP N 41 3580 5223 3810 -203 307 -1779 CA ASP 41 ATOM 334 9.329 33.943 57.613 1.000 27.51 ANISOU 334 CA ASP 41 2705 3858 3891 91 -253 -1061 ATOM 335 С ASP 41 8.107 34.861 57.660 1.000 33.43 ANISOU 335 C ASP 41 3131 3064 6508 32 547 - 1307 ATOM 336 0 ASP . 41 7.034 34.469 58.101 1.000 30.76

							. 61, 623 6, 656 6
ATOM ANISOU ANISOU	33333333333333333333333333333333333333	PPPPPPPPPPPPPPPPPPPPPPPPPPPPPPPPPPPPPP	1493949183746344748186645343336565748781524231225252456642 1411112222222222223333333333333344444444	3 3 0 .8 .2 .7 .3 .0 .7 .2 .3 .9 .9 .1 .3 .9 .0 .2 .1 .8 .2 .9 .0 .7 .4 .8 .2 .3 .9 .9 .1 .3 .9 .9 .1 .1 .8 .2 .9 .0 .7 .4 .8 .2 .2 .9 .0 .7 .4 .8 .2 .2 .8 .2 .9 .0 .7 .4 .8 .2 .2 .8 .2 .9 .0 .7 .4 .8 .2 .2 .8 .2 .2 .8 .2 .2 .8 .2 .2 .2 .2 .2 .2 .2 .2 .2 .2 .2 .2 .2	-24-33403.9164069.013343033333333333333333333333333333333	40       50       10 <td< td=""><td>-1222 -698 -938 1.000 33.37 -739 -501 -571 1.000 34.95 -380 824 -92 1.000 86.76 -10425 588 -1858 1.000 32.71 9 -58 -586 1.000 38.48 1067 -861 -630 1.000 35.83 1136 157 -1162 1.000 37.05 1021 -677 -1532 1.000 98.08 -3208 7500 -2318 1.000 36.08 886 -1119 269 1.000 34.64 656 -275 -698 1.000 32.98 1199 -883 -152 1.000 34.64 656 -275 -698 1.000 32.98 1199 -883 -152 1.000 41.67 225 -1743 953 1.000 38.53 589 -1417 -578 1.000 44.72 28 137 -2137 1.000 53.42 -993 1540 -1338 1.000 50.41 -439 2486 -1725 1.000 59.44 -1284 1632 -2146 1.000 71.33 -4131 6267 -4645 1.000 77.33 -4131 6267 -4645 1.000 77.80 -55 -626 -227 1.000 27.80 -55 -626 -227 1.000 27.80 -55 -626 -227 1.000 27.80 -55 -626 -227 1.000 27.80 -55 -626 -227 1.000 27.80 -55 -626 -227 1.000 27.80 -55 -626 -227 1.000 27.80 -55 -626 -227 1.000 27.80 -55 -626 -227 1.000 27.80 -537 776 -2629 1.000 31.76 -845 792 1217 1.000 47.71 -3576 3333 -2541 1.000 51.56 1956 2240 1382 1.000 41.91 -1455 381 -3537</td></td<>	-1222 -698 -938 1.000 33.37 -739 -501 -571 1.000 34.95 -380 824 -92 1.000 86.76 -10425 588 -1858 1.000 32.71 9 -58 -586 1.000 38.48 1067 -861 -630 1.000 35.83 1136 157 -1162 1.000 37.05 1021 -677 -1532 1.000 98.08 -3208 7500 -2318 1.000 36.08 886 -1119 269 1.000 34.64 656 -275 -698 1.000 32.98 1199 -883 -152 1.000 34.64 656 -275 -698 1.000 32.98 1199 -883 -152 1.000 41.67 225 -1743 953 1.000 38.53 589 -1417 -578 1.000 44.72 28 137 -2137 1.000 53.42 -993 1540 -1338 1.000 50.41 -439 2486 -1725 1.000 59.44 -1284 1632 -2146 1.000 71.33 -4131 6267 -4645 1.000 77.33 -4131 6267 -4645 1.000 77.80 -55 -626 -227 1.000 27.80 -55 -626 -227 1.000 27.80 -55 -626 -227 1.000 27.80 -55 -626 -227 1.000 27.80 -55 -626 -227 1.000 27.80 -55 -626 -227 1.000 27.80 -55 -626 -227 1.000 27.80 -55 -626 -227 1.000 27.80 -55 -626 -227 1.000 27.80 -537 776 -2629 1.000 31.76 -845 792 1217 1.000 47.71 -3576 3333 -2541 1.000 51.56 1956 2240 1382 1.000 41.91 -1455 381 -3537
ATOM :	366	N LYS	45 2 45 3	865 .369	6802 34.195	6256 58.773	-1455 381 $-3537$ 1.000 44.31
ANISOU :	366	CA LYS		768	5427	6639	74 837 - 2985

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ATOM
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       506
           OE2 GLU
                        -17.324 32.041
                     62
                                        56.385 1.000 45.13
ANISOU 506
           OE2 GLU
                     62
                        7600
                                2889
                                        6658
                                               -525
                                                     1698 - 1099
ATOM
       507
           Ν
               LYS
                     63
                        -16.193 25.431
                                        55.345 1.000 25.20
ANISOU 507
           M
               LYS
                     63
                        2470
                                2380
                                        4723
                                               312
                                                     1050 8
MOTA
       508
           CA
               LYS
                     63
                        -15.214 24.369
                                        55.207 1.000 21.62
ANISOU 508
           CA
               LYS
                     63
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                                2894
                                        2712
                                               688
                                                     349 - 446
MOTA
       509
           C
               LYS
                     63
                        -15.708 23.397
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ANISOU 509
           С
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ATOM
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               LYS
                     63
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                                        53.289 1.000 24.17
ANISOU 510
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               LYS
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                                2354
                                        3491
                                               239
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       511
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                     63
ANISOU 511
           CB
               LYS
                     63
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ATOM
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           CG LYS
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ANISOU 512
           CG
               LYS
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ATOM
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           CD LYS
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ANISOU 513
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               LYS
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MOTA
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           CE
               LYS
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ANISOU 514
           CΞ
               LYS
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                                               -317 -286 -792
MOTA
       515
           NZ
               LYS
                     63
                        -12.927 24.614 61.030 1.000 35.00
ANISOU 515
           NZ
               LYS
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                                               64 - 298 - 817
ATOM
       516
           N
               ARG
                     64
                        -17.007 23.112 54.143 1.000 29.82
ANISOU 516
           M
               ARG
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                                2676
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                                        5418
MOTA
       517
           CA
                     64
               ARG
                        -17.521 22.169
                                        53.118 1.000 25.56
ANISOU 517
           CA
               ARG
                     64
                        2396
                                2474
                                        4841
                                               -170 1252 - 962
       518
ATOM
           C
               ARG
                     64
                        -17.417 22.735
                                       51.708 1.000 28.45
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                                               153
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MOTA
       519
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                     64
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                                       50.759 1.000 22.57
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                           1672
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                                                          148 - 395
              СВ
 MOTA
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                       64
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                  ARG
                       64
                           2669
                                    4144
                                            5526
                                                   -809 1483 -1029
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                       64
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 ANISOU 521
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                                                   -2443 1343 -153
 ATOM
         522
              CD
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 ANISOU 522
              CD
                           5723
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 ATOM
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                           -20.759 19.485
                       64
                                            52.714 1.000 77.63
 ANISOU 523
              ΝE
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                       64
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                                                    -4031 -4193 2666
                                            9938
 ATOM
         524
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                  ARG
                       64
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                                            51.696 1.000 60.23
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                                            10644 -1128 -4334 501
 MOTA
         525
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                           -21.424 21.528
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 ANISOU 525
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                       64
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                                    5072
                                            11461 -5082 -3134 - 75
 MOTA
         526
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              NH2 ARG
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 ANISOU 526
              NH2 ARG
                       64
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                                            9178
                                                   -183 -1521 2085
 ATOM
         527
              Ν
                  ALA
                       65
                           -17.624 24.041
                                            51.515 1.000 26.71
 ANISOU 527
              И
                  ALA
                       65
                           1907
                                   2770
                                            5472
                                                   189
                                                          936 - 556
 MOTA
         528
              CA
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                       65
                           -17.522 24.661
                                            50.199 1.000 24.91
 ANISOU 528
              CA
                 ALA
                       65
                           1798
                                    2379
                                            5288
                                                   280
                                                          417 - 754
 MOTA
         529
              C
                  ALA
                       65
                           -16.109 24.575
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 ANISOU 529
              С
                  ALA
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                                    2408
                                            4071
                                                   597,
                                                          155 - 626
 ATOM
         530
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                                            48.381 1.000 24.13
 ANISOU 530
              0
                  ALA
                       65
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                                    3076
                                                         -220 - 485
                                            3964
                                                   224
 ATOM
         531
              CB
                       65
                 ALA
                           -18.023 26.096
                                            50.221 1.000 31.78
 ANISOU 531
              СВ
                 ALA
                       65
                           3096
                                   2984
                                            5993
                                                   1337
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 ATOM
         532
             N
                  VAL
                       66
                           -15.098 24.306
                                            50.426 1.000 19.29
 ANISOU 532
             N
                  VAL
                       66
                           1836
                                   1880
                                            3614
                                                   466
                                                          360 - 541
 MOTA
         533
             CA
                  VAL
                       66_ -13.723 24.167
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- ANISOU 533
             CA
                  VAL
                       66
                           1636
                                   1653
                                            3616
                                                   204
                                                          79 - 487
 ATOM
        534
              C
                  VAL
                       66
                           -13.166 22.767
                                            50.248 1.000 15.18
 ANISOU 534
              С
                  VAL
                       66
                           1516
                                   1638
                                            2613
                                                   120
                                                          126 - 571
 MOTA
        535
                           -11.959 22.623
1567 2071
              0
                  VAL
                       66
                                            50.353 1.000 17.63
 ANISOU 535
             \circ
                  VAL
                       65
                                            3060
                                                   217
                                                         -106 - 317
 MOTA
        536
             СВ
                 VAL
                       66
                           -12.784 25.277
                                            50.437 1.000 18.91
 ANISOU 536
             CB
                 VAL
                       66
                           2175
                                   1576
                                            3433
                                                   183 -135 - 598
 MOTA
        537
             CG1 VAL
                       65
                           -13.139 26.627
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 ANISOU 537
              CG1 VAL
                       66
                           2067
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                                            4010
                                                   219
                                                          593 - 83
 ATOM
                           -12.736 25.373
        538
             CG2 VAL
                       66
                                            51.945 1.000 21.61
 ANISOU 538
             CG2 VAL
                       66
                           2689
                                   2066
                                            3455
                                                   102
                                                          22 - 603
 MOTA
         539
             N
                  THR
                           -14.048 21.792
                       67
                                            50.343 1.000 18.30
 ANISOU 539
             Ν
                  THR
                       67
                           1761
                                   1614
                                            3577
                                                   -20
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 ATOM
         540
                       67
             CA
                 THR
                           -13.673 20.403
                                            50.563 1.000 17.18
 ANISOU 540
             CA
                  THR
                       67
                           1927
                                   1656
                                            2946
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 MOTA
        541
              C
                  THR
                       67
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 ANISOU 541
              C
                  THR
                       67
                           1763
                                   1742
                                            2773
                                                   21 27 - 467
 ATOM
        542
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                  THR
                       67
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 ANISOU 542
             0
                  THR
                       67
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                                   2211
                                            2929
                                                   73 -86 - 383
 ATOM
        543
             CB
                 THR
                       67
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 ANISOU 543
                       67
             CВ
                 THR
                           2202
                                    2014
                                            2827
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                                                          224 - 492
 MOTA
        544
              OG1 THR
                       67
                           -14.060 20.554
                                            52.961 1.000 20.14
 ANISOU 544
              OG1 THR
                       67
                           2481
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                                                   -108
                                                         155 - 468
 MOTA
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              CG2 THR
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 ANISOU 545
             CG2 THR
                       67
                           2393
                                    2016
                                            3203
                                                   29 -86 -235
 MOTA
        546
             \mathbf{N}
                  SER
                       68
                           -13.030 18.818
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 ANISOU 546
             N
                  SER
                       68
                           1612
                                    1720
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 ATOM
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                       68
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 ANISOU 547
              CA
                  SER
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                           1508
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 MOTA
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              C
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- 31 -ATOM 550 CB SER 68 -11.958 17.303 47.257 1.000 17.84 ANISOU 550 CB SER 68 1459 2139 3182 -87 647 -313 ATOM 551 OG SER 68 -10.998 18.259 46.904 1.000 17.21 ANISOU 551 OG SER 68 1659 1987 2893 -75 364 -49 69 -14.929 69 1574 69 -15.877 69 1428 MOTA 552 N PRO -14.929 16.284 47.054 1.000 15.89 ANISOU 552 N PRO 1574 1661 2803 -201 -103 - 280 553 CA PRO -15.877 15.182 47.339 1.000 16.42 ATOM ANISOU 553 CA PRO 1903 2908  $-251 \quad -148 \quad -218$ 69 554 C ATOM -15.168 13.889 47.684 1.000 17.22 PRO PRO 69 1633 1578 3331 -199 266 -PRO 69 -15.794 12.997 48.287 1.000 18.35 ANISOU 554 C -199 266 -424 555 O 69 1815 1760 3399 -365 232 -376 69 -16.712 15.057 46.060 1.000 16.75 69 1354 2279 2733 -360 155 -729 ANISOU 555 O PRO ATOM 556 CB PRO ANISOU 556 CB PRO ATOM 557 CG PRO 69 -15.799 15.637 45.008 1.000 16.72 ANISOU 557 CG PRO 69 1553 1971 2827 -359 38 -45 2827 ATOM 558 CD PRO 69 1553 1971 2827 -359 38 -452
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ANISOU 559 N VAL 70 1716 1764 3384 -89 292 -215
ATOM 560 CA VAL 70 -13.100 12.594 47.824 1.000 17.34
ANISOU 560 CA VAL 70 1763 1851 2974 -20 260 -196
ATOM 561 C VAL 70 -11.995 13.142 48.720 1.000 17.59 38 - 452 70 1716 1764 3384 -89 292 -2 70 -13.100 12.594 47.824 1.000 17.34 70 1763 1851 2974 -20 260 -2 70 -11.995 13.142 48.720 1.000 17.59 70 2207 1686 2788 -180 159 -142 70 -11.431 14.186 48.389 1.000 18.59 ANISOU 561 C VAL ATOM 562 O VAL ANISOU 562 O VAL 70 1794 1688 3581 -4 9 152 ATOM 563 CB VAL 70 -12.429 11.757 46.724 1.000 18.10 ANISOU 563 CB VAL 70 1922 1756 3199 -353 560 -446 ATOM 564 CG1 VAL 70 -13.441 10.754 46.213 1.000 20.54 ANISOU 564 CG1 VAL 70 1927 2611 3268 -369 76 -663 ATOM 565 CG2 VAL 70 -11.760 12.608 45.642 1.000 17.65 ANISOU 565 CG2 VAL ATOM 566 N PRO 70 2379 1806 2520 145 9 1 0 71 -11.697 12.466 49.815 1.000 16.21 71 1653 1810 2695 -34 464 -ANISOU 566 N PRO 2695 -34 464 -156 71 -10.839 13.091 50.833 1.000 17.32 71 1795 1931 2854 -121 184 -12 71 -9.356 12.804 50.590 1.000 17.67 MOTA 567 CA PRO ANISOU 567 CA PRO 568 C PRO ATOM ANISOU 568 C PRO /1 1865 1927 2921 46 -57 1 5 6 71 -8.585 12.223 51.350 1.000 20.57 ATOM 569 O PRO ANISOU 569 O PRO 71 2218 2247 3350 424 28 4 7 4
ATOM 570 CB PRO 71 -11.362 12.458 52.117 1.000 19.76
ANISOU 570 CB PRO 71 2976 1862 2668 -347 479 -304
ATOM 571 CG PRO 71 -11.721 11.056 51.670 1.000 19.08
ANISOU 571 CG PRO 71 2838 1805 2608 -267 259 -234
ANISOU 572 CD PRO 71 -12.323 11.220 50.286 1.000 17.97
ANISOU 572 CD PRO 71 2314 1974 2538 -390 451 -167
ANISOU 573 N THR 72 -8.894 13.338 49.446 1.000 17.15
ANISOU 573 N THR 72 1677 2231 2610 -215 -17 -165
ANISOU 574 CA THR 72 -7.573 13.012 48.935 1.000 16.83
ANISOU 574 CA THR 72 1721 1863 2810 -60 -134 -472
ANISOU 575 C THR 72 -6.490 14.000 49.358 1.000 15.20
ANISOU 575 C THR 72 -6.490 14.000 49.358 1.000 15.20
ANISOU 576 O THR 72 -5.320 13.729 49.104 1.000 17.49
ANISOU 576 O THR 72 -5.320 13.729 49.104 1.000 17.49 ANISOU 569 O PRO 71 2218 2247 3350 28 4 7 4 577 CB THR 72 1776 1961 2908 -61 -31 -225 577 CB THR 72 -7.533 12.971 47.399 1.000 16.18 578 OG1 THR 72 1552 1848 2748 -146 36 365 ANISOU 576 O THR 72 1776 MOTA ANISOU 577 578 ATOM OG1 THR 72 -8.091 14.238 47.005 1.000 17.81 ANISOU 578 OG1 THR 72 1856 1880 3031 -34 115 -191 ATOM 579 CG2 THR 72 -8.338 11.816 46.825 1.000 17.49 ANISOU 579 CG2 THR 72 1953 2087 2605 -550 181 -329 ATOM 580 MET 73 -6.877 15.098 49.987 1.000 17.78

- 32 -ANISOU 580 N 73 2057 1748 MET 2951 -58 -254 - 426ATOM 581 CA MET 73 -5.867 16.117 50.394 1.000 16.58 ANISOU 581 CA MET 73 1708 1796 2797 88 -302 -340 MOTA 582 -5.073 C MET 73 16.618 49.198 1.000 16.65 ANISOU 582 С MET 73 1514 1787 3027 241 -162 - 420MOTA 583 0 MET 73 -3.911 17.039 49.292 1.000 19.39 ANISOU 583 0 MET 73 1705 2313 3348 -112 -240 - 540 СВ ATOM 584 MET 73 -4.925 15.531 51.469 1.000 20.56 ANISOU 584 CB MET 73 3083 345 -507 - 286 2099 2629 73 MOTA 585 CG MET -5.703 52.715 1.000 30.33 15.154 ANISOU 585 CG 73 MET 3008 5133 3384 -69 -609 1 0 2 7 MOTA 586 SD MET 73 -4.692 14.263 53.891 1.000 36.13 ANISOU 586 MET 73 SD 4121 5050 4558 336 -918 1596 ATOM 587 CE MET 73 -3.165 13-987 53.082 1.000 58.07 ANISOU 587 CE MET 2810 73 8820 10435 975 -1592 -3138 MOTA 588 N ARG 48.025 1.000 16.83 74 -5.687 16.632 ANISOU 588 N ARG 74 1699 2982 -6 -211 131 1714 ÇA ATOM 589 ARG 74 -5.099 17.215 46.817 1.000 15.87 ANISOU 589 CAARG 74 1365 1618 3046 -17 52 - 325 MOTA 590 C ARG 74 -5.359 18.714 46.761 1.000 14.22 ANISOU 590 С ARG 74 1484 1651 2269 -32 - 42 141 591 0 ATOM ARG 74 -4.47219.488 46.353 1.000 15.45 ANISOU 591 0 ARG 74 1525 1758 2586 -12 -46 - 73 MOTA 592 CB 74 ARG 16.530 45.566 1.000 15.68 -5.675 ANISOU 592 CB ARG 74 1330 1667 2959 160 -14 - 311ATOM 593 CG 74 ARG -4.890 16.941 44.299 1.000 16.46 ANISOU 593 CG ARG 74 1325 1870 3059 -175 55 - 395 ATOM 594 CD ARG 74 16.396 43.072 1.000 16.37 ANISOU 594 CD1533 ARG 74 1789 2899 -181 -8 -177 ATOM 595 16.601 41.857 1.000 19.21 NEARG 74 -4.840ANISOU 595 ΝE ARG 74 2289 1990 3020 -142 241 -156 ATOM 596 CZARG 74 -4.944 17.626 41.039 1.000 17.00 ANISOU 596 ARG CZ74 1545 2351 2562 -67 26 - 147MOTA 597 NH1 ARG 74 -5.878 18.573 41.213 1.000 18.00 ANISOU 597 NH1 ARG 74 1818 2383 2638 51 -66 - 220 ATOM 598 NH2 ARG 17.703 39.987 1.000 20.50 74 -4.144ANISOU 598 NH2 ARG 74 2285 2972 2532  $-110 \cdot 310 - 387$ 75 MOTA 599 N ARG -6.579 19.151 47.101 1.000 15.28 ANISOU 599 ARG 75 1755 N 1544 2507 137 340 - 173ATOM 600 CA ARG 75 -6.999 20.550 46.980 1.000 14.68 ANISOU 600 CA 1679 ARG 75 162.7 2272 236 98 - 150 ATOM 601 C ARG 75 -7.95620.869 48.122 1.000 14.75 ANISOU 601 С 75 ARG 1445 1747 2414 124 133 - 233 ATOM 602 0 -8.760 19.989 48.460 1.000 18.12 ARG 75 ANISOU 602 0 ARG 75 1677 2109 3101 -156 458 -433 MOTA 603 CB ARG 75 -7.747 20.804 45.668 1.000 15.59 ANISOU 603 CB ARG 75 1577 2030 2317 · 1 46 - 106 ATOM 604 CG ARG 75 -6.848 20.634 44.441 1.000 15.63 ANISOU 604 CG ARG 75 1495 2110 2334 9 147 2 2 0 MOTA 605 75 CDARG -5.71221.618 44.334 1.000 15.59 ANISOU 605 CD ARG 75 1658 1792 2475 11 130 - 10 MOTA 606 ΝE 75 ARG -5.061 21.601 43.011 1.000 15.25 ANISOU 606 NΕ ARG 75 1421 1779 2596 227 122 ATOM 607 CZARG 75 -3.957 20.865 42.732 1.000 14.90 ANISOU 607 CZARG 75 1079 2361 71 -86 2 4 2 2221 ATOM 608 75 NH1 ARG -3.40520.091 43.664 1.000 16.18 ANISOU 608 NH1 ARG 75 1804 1722 -134 -387 3 3 7 2623 ATOM 609 NH2 ARG 75 -3.41820.940 41.518 1.000 15.83 ANISOU 609 NH2 ARG 75 1677 2107 2232 -193 221 0 ATOM 610 N GLY 76 -7.895 22.086 48.651 1.000 16.06 ANISOU 610 Ν GLY 76 1686 1904 2513 109 220 - 464

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- 33 -
                       611 CA GLY 76 -8.858 22.532 49.637 1.000 16.67
611 CA GLY 76 1650 2260 2425 -70 199 -6
612 C GLY 76 -8.602 22.002 51.036 1.000 16.32
612 C GLY 76 1584 2014 2602 -126 268 -3
613 O GLY 76 -7.469 21.651 51.370 1.000 16.87
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      ATOM
      ANISOU 612 C
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      ATOM
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614 N PHE 77 -9.643 22.025 51.863 1.000 16.88
      ANISOU 613 O
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                                  CA PHE 77
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                                                                                                                                        328 -114
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                                            PHE 77 1855 2248
     ANISOU 616 C
                                                                                                           2600 -68
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77 -12.079 20.991 57.300 1.000 25.09
     ANISOU 622 CE1 PHE
                                                      77 -12.079 20.991 57.300 1.000 25.09

77 2967 4120 2447 -501 625 -77 -11.175 21.523 58.207 1.000 23.79

77 2263 3681 3095 -1 376 - 756

78 -9.022 19.631 54.490 1.000 17.64

78 1616 2161 2925 37 336 1

78 -9.296 18 270
                      623 CE2 PHE
     ATOM
ATOM 623 CE2 PHE
ANISOU 623 CE2 PHE
ATOM 624 CZ PHE
ANISOU 624 CZ PHE
ATOM 625 N THR
ANISOU 625 N THR
ATOM 626 CA THR
ANISOU 626 CA THR
ANISOU 627 C THR
ANISOU 627 C THR
ANISOU 628 O THR
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-9.296 18.279 54.983 1.000 18.12
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THR 78 -9.291 18.316 56.505 1.000 18.66
                                                                                                          2717 -157 624 - 28
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                   628 O THR 78 -8.335 18.821 57.095 1.000 21.42
U 628 O THR 78 2158 2883 3098 -432 90 17
    ATOM
    ANISOU 628 O THR 78 2158
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                      630 OG1 THR
                                                       78 -8.027 17.392 53.104 1.000 21.18
    ANISOU 630 OG1 THR
                                                       78 2544 2671
                                                                                                          2833 160
                                                                                                                                           317 - 773
    ATOM
                     631
                                CG2 THR
                                                      78 -8.735 15.832 54.800 1.000 26.65
78 3759 2227 4141 -275 853 -618
   ATOM 631 CG2 THR 78 -8.735 15.832 54.800 1.000 26.65

ANISOU 631 CG2 THR 78 3759 2227 4141 -275 853 -618

ATOM 632 N GLY 79 -10.311 17.804 57.181 1.000 20.36

ANISOU 632 N GLY 79 2669 2379 2690 -670 630 -144

ATOM 633 CA GLY 79 -10.344 17.679 58.623 1.000 25.96

ANISOU 633 CA GLY 79 3871 3249 2745 -790 576 3 7 5

ATOM 634 C GLY 79 -10.029 16.238 59.039 1.000 39.70

ANISOU 634 C GLY 79 6407 3542 5135 -1658 -1944 151

ATOM 635 O GLY 79 -10.623 15.303 58.491 1.000 31.02

ANISOU 635 O GLY 79 4327 3187 4272 -404 419 -75

ATOM 636 N LEU 80 -9.069 16.055 59.936 1.000 36.07

ANISOU 636 N LEU 80 4380 4536 4788 1381 -564 -835
   ATOM 631 CG2 THR
ANISOU 631 CG2 THR
ATOM 632 N GLY
ANISOU 632 N GLY
ATOM 633 CA GLY
ANISOU 633 CA GLY
ANISOU 633 CA GLY
ANISOU 634 C GLY
                                                                                                          5135 -1658 -1944 1511
   ANISOU 636 N LEU 80 4380 4536 4788 1381 -564 -835 ATOM 637 CA LEU 80 -8.634 14.713 60.340 1.000 32.52 ANISOU 637 CA LEU 80 3640 4083 4632 611 -502 -898 ATOM 638 C LEU 80 -9.131 14.311 61.716 1.000 39.82 ANISOU 638 C LEU 80 5051 4652 5428 -128 418 -538 ATOM 639 O LEU 80 -9.998 14.963 62.305 1.000 37.05 ANISOU 639 O LEU 80 5057 3807 5213 -292 666 8 7 ATOM 640 CB LEU 80 -7.122 14.580 60.265 1.000 38.36 ANISOU 640 CB LEU 80 3821 5456 5299 1568 -33 -1404 ATOM 641 CG LEU 80 5057 3821 5456
                                                                                                                         1568 -33 -1406
    ATOM 641 CG LEU
                                                        8.0
                                                                  -6.488 14.753 58.883 1.000 38.27
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- 34 -ANISOU 641 CG LEU 80 3714 5900 4926 725 -288 - 2588 80 -5.007 14.359 58.948 1.000 45.41 642 CD1 LEU ANISOU 642 CD1 LEU 80 2579 8505 6170 -1092 -76 3 ATOM 643 CD2 LEU 8.0 -7.170 13.856 57.854 1.000 40.75 ANISOU 643 CD2 LEU 8 0 4296 5601 5587 372 -1965 -1793 ATOM 644 N SER 98 -6.459 17.442 63.930 1.000 36.72 ANISOU 644 Ν SER 98 3404 6429 4118 -2114 -698 1948 645 CASER 98 -5.629 17.877 62.824 1.000 39.59 CA SER ANISOU 645 98 6031 5376 3635 -449 383 2177 ATOM 646 C SER 98 -6.402 18.372 61.610 1.000 29.89 ANISOU 646 С SER 98 3806 3509 4040 141 640 1204 ATOM 647 -7.474 17.856 0 98 SER 61.304 1.000 38.27 ANISOU 647 0 SER 98 4936 4300 5303 -1107 395 885 ATOM 648 CB SER 98 -4.694 16.739 62.358 1.000 44.06 ANISOU 648 CВ SER 98 3175 7425 6141 633 -753 2704 MOTA 649 OG SER 98 -3.672 17.368 61.583 1.000 46.84 ANISOU 649 ОG 98 SER 3497 7797 6502 95 -408 2418 ATOM 650 Ν MET 99 -5.829 19.317 60.869 1.000 28.56 ANISOU 650 M MET 99 5029 3458 2365 -1080 -550 5 4 6 ATOM CA MET 651 99 -6.426 19.941 59.700 1.000 21.44 CA MET ANISOU 651 99 2284 3549 2315 -182 157 132 652 C < MET -5.376 20.229 99 58.624 1.000 19.16 ANISOU 652 С MET 99 2306 2592 2382 -433 60 1 3 7 MOTA 653 0 MET 99 -4.232 20.575 58.930 1.000 23.34 ANISOU 653 0 MET 99 2489 3920 2460 -773 225 -410 ATOM 654 CB MET 99 -7.164 21.209 60.105 1.000 25.20 ANISOU 654 ·CB MET 99 3172 3375 3028 -572 661 -547 ATOM 655 CG MET 99 = -8.481 20.965 60.872 1.000 25.85 ANISOU 655 CG MET 99 3172 3862 2787 -275 739 - 782 ATOM 656 99 SD MET -9.251 22.517 61.389 1.000 32.21 ANISOU 656 SD MET 99 4405 3750 4083 -133 1580 - 568 ATOM 657 CE MET 99 -8.884 22.461 63.145 1.000 76.12 ANISOU 657 99 14782 11538 2603 -3321 3478 -100 -5.778 20.094 57.361 1.000 18.85 СE MET 99 -3321 3478 -3241 ATOM 658 CYS Ν ANISOU 658 N CYS 100 2434 2443 100 2434 2443 2285 -160 93 1 9 100 -4.868 20.333 56.234 1.000 18.55 -160 93 1 9 4 ATOM 659 CA CYS ANISOU 659 CA CYS 100 2251 2380 2418 92 127 2 3 6 100 -5.496 21.312 55.228 1.000 16.26 MOTA 660 C CYS ANISOU 660 C CYS 100 1826 2031 2321 110 329 2 100 -6.728 21.308 55.071 1.000 17.69 ATOM 661 O CYS ANISOU 661 0 CYS 100 1741 2395 2586 -69 154 -104 100 -4.604 18.982 55.545 1.000 18.46 100 1741 MOTA 662 СB CYS ANISOU 662 CB CYS 100 2822 2081 2111 98 118 5 1 1 ATOM 663 100 -3.243 18.974 54.329 1.000 22.76 SG CYS ANISOU 663 CYS SG 100 2622 2968 3058 307 391 1 0 664 101 -4.697 22.069 54.498 1.000 17.49 Ν TYR ANISOU 664 N TYR 101 1839 2473 2332 46 291 2 2 4 ATOM 665 CA- TYR 101 -5.117 22.874 53.373 1.000 15.38 ANISOU 665 CA TYR 101 1946 1939 1960 -50 90 - 262 ATOM 666 C TYR 101 -4.102 22.594 52.245 1.000 13.65 ANISOU 666 С TYR 101 1676 1967 -2 -123 -151 52.475 1.000 15.95 1543 MOTA 667 0 TYR 101 -2.896 22.629 ANISOU 667 0 TYR 101 1611 2231 2217 -43 -232 - 212 MOTA 668 СB TYR 101 -5,122 24.382 53.739 1.000 19.02 ANISOU 668 CB TYR 101 2816 2082 2328 234 48 - 519 ATOM 669 CG TYR 101 -5.617 25.109 52.498 1.000 17.85 ANISOU 669 CG TYR 101 2084 1895 2804 18 -26 -231 ATOM 670 CD1 TYR 101 -6.964 25.134 52.171 1.000 18.25 ANISOU 670 CD1 TYR 101 2042 1596 3298 29 28 - 496 671 CD2 TYR 101 -4.730 25.778 51.658 1.000 17.77 ANISOU 671 CD2 TYR 101 2037 1611 3106 -46 -125 - 127

- 35 -672 CE1 TYR 101 -7.406 25.796 51.036 1.000 19.63 MOTA CE1 TYR 101 1977 ANISOU 672 1776 3704 88 -241 -221 673 CE2 TYR 101 -5.147 26.386 50.478 1.000 20.46 ANISOU 673 CE2 TYR 101 2060 2608 3108 239 40 182 ATOM 674 CZTYR 101 -6.504 26.392 50.166 1.000 20.29 ANISOU 674 CZTYR 101 2187 2397 3127 -73 -353 - 260MOTA 675 OΗ TYR 101 -6.932 26.995 49.000 1.000 23.34 ANISOU 675 ОН TYR 101 2790 2555 3523 -3 -641 676 N MOTA SER 102 -4.648 22.210 51.097 1.000 14.60 ANISOU 676 N SER 102 1618 1890 2041 -61 -109 - 477 21.792 49.980 1.000 14.52 677 CA SER 102 -3.797 ANISOU 677 CA SER 102 1684 1802 2030 -108 62 - 276 678 C 102 -4.011 22.670 48.747 1.000 14.99 ATOM SER ANISOU 678 C SER 102 1545 1790 2361 -296 -41 679 0 ATOM 23.105 48.477 1.000 16.73 SER 102 -5.167 ANISOU 679 O SER ATOM 680 CB SER ANISOU 680 CB SER ATOM 681 OG SER 102 1589 2342 2425 2 128 -102 -4.163 20.340 49.593 1.000 13.82 102 1692 2013 174 9 -138 1548 102 -3.996 19.476 50.720 1.000 16.06 ANISOU 681 OG SER 102 1886 2066 2153 97 -121 6 3 ATOM 682 N 103 -2.978 22.775 47.920 1.000 14.47 MET ANISOU 682 N MET 103 1568 1724 2206 51 -59 1 5 2 683 CA MET MOTA 103 -3.102 23.552 46.687 1.000 16.58 ANISOU 683 CA MET 103 2194 1933 2173 331 -74 253 103 -2.150 23.013 45.608 1.000 14.41 MOTA 684 C MET ANISOU 684 C MET 103 1598 1793 2083 -202 -210 6 3 685 0 ATOM 103 -1.157 22.347 45.920 1.000 16.24 MET ANISOU 685 O MET ATOM 686 CB MET ANISOU 686 CB MET 
 103
 1527
 2384
 2259
 -61
 -23
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 -2.716
 25.004
 46.835
 1.000
 28.78
 -23 468 103 6537 -207 3 6 6 1318 3081 859 MOTA 687 CG 103 -3.258 25.986 47.801 1.000 22.60 MET CG ANISOU 687 MET 103 2531 2157  $3900 \sim -161 -57 -291$ 688 SD ATOM MET 103 -2.338 27.505 47.506 1.000 20.60 SD ANISOU 688 MET 103 2499 1927 3400 -4 -164 -226 MOTA 689 CE MET 103 -2.587 27.945 45.804 1.000 21.63 ANISOU 689 CE 103 2319 MET 3300 2601 308 209 - 236 ATOM 690 N GLY 104 - 2.43923.430 44.378 1.000 15.44 ANISOU 690 N GLY 104 1468 2228 2169 -68 -120 1 6 4 691 CA GLY ATOM 104 -1.511 23.199 43.276 1.000 16.13 ANISOU 691 CA GLY 104 1688 2202 2241 42 65 4 6 9 692 C ATOM GLY 104 -1.583 24.355 42.294 1.000 15.76 ANISOU 692 C ATOM 693 O ANISOU 693 O GLY 104 1706 1997 2286 -32 -194 3 8 8 104 -1.987 GLY25.478 42.653 1.000 19.06  $\operatorname{\mathsf{GLY}}$ 104 1953 2032 3256 -71 144 3 3 3 N ATOM 694 THR 105 -1.151 24.092 41.054 1.000 16.73 N ANISOU 694 THR 105 1685 2385 2287 -375 -55 515 ATOM 695 CA THR 105 -1.115 25.205 40.094 1.000 17.06 ANISOU 695 CA THR 105 1725 2390 2369 -231 -148 5 7 7 696 C ATOM THR 105 -2.513 25.631 39.635 1.000 19.55 ANISOU 696 C 105 1768 THR 1817 3842 -160 -346 5 2 5 ATOM 697 0 THR 105 -2.680 26.703 39.059 1.000 22.41 ANISOU 697 O 105 2262 THR 2116 4136 -119 -520 8 4 2 698 CB THR ATOM 105 -0.301 38.840 1.000 17.57 24.857 ANISOU 698 CB THR 105 1759 2877 2038 -394 -343 3 7 7 MOTA 699 OG1 THR 105 -0.865 23.675 38.217 1.000 18.66 ANISOU 699 OG1 THR 105 2035 2449 2607 -140 -458 4 1 6 700 CG2 THR 105 1.155 24.590 39.178 1.000 18.95 ANISOU 700 CG2 THR 105 1748 2853 2601 -105 -248 2 9 6 ATOM 701 N ALA 106 -3.507 24.751 39.741 1.000 16.52 ANISOU 701 N ALA 106 1596 2293 2389 -180 -1 2 9 8 702 ATOM C.A. ALA 106 -4.846 25.035 39.218 1.000 16.59

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ANISOU ATOM		CA	ALA		1692	1952	2660	-214 -209 2 4 3
ANISOU	703	C	ALA		-5.848	24.142	39.923	1.000 17.52
ATOM	704	С	ALA	106		1821	3186	26 -66 5 5 5
		0	ALA	106	-5.479	23.323	40.805	1.000 17.88
ANISOU ATOM		0	ALA	106	2038	2087	2668	59 -51 3 8 8
ANISOU	705	CB	ALA	106	-4.862	24.838	37.713	1.000 20.31
ATOM	706	CB	ALA	T06	2331	2764	2620	-197 -403 4 4 0
ANISOU		N N	ASP		-7.149	24.329	39.717	1.000 18.00
ATOM	707	CA	ASP	107	1576 `	2208	3057	-77 -120 4 9
ANISOU		CA	ASP ASP	107	-8.217	23.535	40.344	1.000 17.46
ATOM	708	C	ASP		1563	2191	2881	-83 -472 3 6 3
ANISOU		C	ASP	107	-8.173 1825	23.753	41.859	1.000 17.74
ATOM	709	Õ	ASP	107	-8.458	2044	2869	447 -269 3 6 2
ANISOU		Ö	ASP	107	1994	22.854 2230	42.650	1.000 18.95
ATOM	710	ČВ	ASP	107	-8.089	22.044	2974	167 -133 4 0 2
ANISOU	710	СВ	ASP	107	2213	2300	2942	1.000 19.62
ATOM	711	CG	ASP	107	-8.370	21.842		-394 -727 1 7 3
ANISOU		CG	ASP	107	1952	3093	2862	1.000 20:81 -138 -532 - 14
ATOM	712		ASP -	107	-9.369	22.369		1.000 25.84
ANISOU			ASP	107	2524	3967	3327	222 -1149 - 240
ATOM	713		ASP		-7.544	21.168	37.844	1.000 25.86
ANISOU	713		ASP	107	3314	2989	3523	391 -91 -89
ATOM ANISOU	714	N	ASN	108	-7.893	24.962	42.298	1.000 18.18
ATOM	714 715	N CA	ASN	108	2049	2075	2786	509 189 153
ANISOU	715	CA	ASN ASN	108	-7.831	25.263	43.740	1.000 17.10
ATOM	716	C	ASN	108	1804 -9.158	1977	2715	266 291 327
ANISOU		C	ASN	100	1705	25.716 2061	44.314	1.000 17.11
ATOM	717	Ō	ASN		-10.103	2001	2734	367 44 1 4 9
ANISOU	717	0	ASN	108	2066	2377	3430	1.000 20.72 759 -248 245
ATOM	718	CB	ASN	108	-6.799	26.379		759 -248 2 4 5 1.000 19.90
ANISOU		СB	ASN	108	1770	2308	3483	186 298 -171
ATOM	719	CG	ASN	108	-5.400	25.862		1.000 17.24
ANISOU		CG	ASN	108	1709	2212	2628	200 68 1 8 4
ATOM	720		ASN	108	-4.986	24.850		1.000 17.42
ANISOU ATOM	720 721	OD1			2003	1984	2631	109 11 - 62
ANISOU		ND2		108	-4.644	26.487	42.834	1.000 18.41
ATOM	722	N	LEU	108	2083 -9.308	2326	2587	-82 300 - 18 _
ANISOU	722		LEU	109	1795	25.509	45.607	1.000 18.09
ATOM	723	CA	LEU	109	-10.532	2294	2786	349 344 1 0
ANISOU	723	CA		109	1763	2200	3296	1.000 19.11 14 476 - 598
MOTA	724	С	LEU		-10.169	26 790		1.000 17.40
ANISOU			LEU	109	1682	1937	2990	251 129 - 207
ATOM	725	0	LEU	109	-9.443	26.423		1.000 21.18
ANISOU	725		LEU	109	2443	1922	3684	174 -520 2
ATOM ANISOU	726	CB	LEU	109	-11.100	24.504		1.000 17.10
ATOM	726 727	CB	LEU	109	1888	2142	2469	199 426 -630
ANISOU	727	CG CG	LEU	109	-11.520		45.944	1.000 18.07
ATOM	728	CD1	LEU	109	2515	1943	2409	190 -198 - 363
ANISOU	728	CD1	LEU	109	-11.895 2842		46.654	1.000 20.06
ATOM	729	CD2	LEU	109	-12.630	2406	2375	-331 -175 - 200
ANISOU		CD2	LEU	109	3481	2892	45.035 3217	1.000 25.24
MOTA	730	N	PHE		-10.609	28.036		306 -992 -111 1.000 17.25
	730	И	PHE	110	1584	1926	3045	272 184 -132
ATOM	731	CA	PHE	110	-10.235	29.071		1.000 18.20
	731	CA	PHE	110	1751	1816	3346	169 221 -160
ATOM ANISOU	732	C	PHE	110	-11.409	29.567		1.000 19.93
T117200	132	С	PHE	110	2077	1609	3886	71 650 - 335

- 37 -733 0 110 -12.433 29.948 48.494 1.000 24.64 ATOM PHE ANISOU 733 O PHE 110 2051 2461 4851 612 328 - 779 ATOM 734 110 -9.607 30.243 47.520 1.000 19.92 CB PHE CB PHE ANISOU 734 110 2367 1876 3324 224 619 - 93735 ATOM CG PHE110 -8.380 29.986 46.688 1.000 19.47 ANISOU 735 CG PHE CD1 PHE 110 2009 2209 3179 -321 327 MOTA 736 110 -7.177 29.680 47.287 1.000 20.59 ANISOU 736 CD1 PHE 110 2071 2080 3674 -274 236 ATOM 737 110 -8.437 30.035 45.299 1.000 20.19 CD2 PHE ANISOU 737 CD2 PHE 110 2557 1914 3200 112 543 ATOM 738 CE1 PHE 110 -6.034 29.454 46.559 1.000 21.06 ANISOU 738 CE1 PHE 110 2020 2309 3673 -386 165 -110 -7.277 29.811 44.547 1.000 20.77 -386 165 -622 CE2 PHE ATOM 739 ANISOU 739 CE2 PHE 110 2495 2138 3257 197 504 - 398 110 -6.081 29.518 740 CZ PHE MOTA 45.175 1.000 22.42 ANISOU 740 CZ PHE 110 2747 2092 3678 531 339 - 357 111 -11.238 29.718 50.416 1.000 22.11 ATOM 741 N PRO ANISOU 741 N PRO 111 2250 2153 3996 -72 871 - 620 CA PRO CA PRO 111 -12.237 30.389 51.195 1.000 28.23 ATOM 742 ANISOU 742 111 3895 2210 4621 698 1514 - 671 ATOM 743 C PRO 111 -12.333 31.866 50.784 1.000 30.57 ANISOU 743 С PRO 111 4528 2026 5061 410 410 -1041 ATOM 744 PRO 111 -11.390 32.340 50.115 1.000 31.71 0 < ANISOU 744 0 PRO 111 4040 2236 5774 -179 -597 - 12 745 CB PRO 111 -11.799 30.250 52.627 1.000 33.20 ANISOU 745 CB PRO 111 5609 2702 4303 671 1671 - 790 ATOM 746 CG 111 -10.646 29.326 52.647 1.000 26.04 PRO ANISOU 746 .CG PRO 111 2742 3835 3316 -931 1324 - 192 ATOM 747 CDPRO 111-10.161 29.149 51.230 1.000 22.15 ANISOU 747 CD PRO 111 2587 2307 -471 541 -623 3522 ATOM 748 112 -13.337 32.641 51.150 1.000 42.13 N SER ANISOU 748 N SER 112 7176 2716 6115 2074 1731 - 526 ATOM 749 112 -13.368 34.026 50.672 1.000 44.05 CASER ANISOU 749 CA SER 112 6799 2255 7684 1107 -485 -826 750 MOTA SER 112 -13.262 34.157 49.149 1.000 68.28 ANISOU 750 C SER 112 13632 4498. 7812 -1855 -2077 1301 ATOM 751 0 112 -12.347 34.825 48.646 1.000 95.18 SER ANISOU 751 O 112 15991 11425 8747 -4337 -70 1 112 -12.493 35.069 51.349 1.000 39.31 SER 8747 -4337 -70 1985 ATOM 752 CB SER ANISOU 752 CB SER 112 2247 4535 8153 580 1662 - 1437 753 OG ATOM SER 112 -11.474 34.624 52.213 1.000 37.49 ANISOU 753 OG SER 112 7213 2453 4579 806 747 -1152 ATOM 754 N ASP 114 -9.515 37.322 49.945 1.000 36.40 ANISOU 754 N ASP 114 3476 2118 8237 1254 403 1484 ATOM 755 CA ASP ANISOU 755 CA ASP ATOM 756 C ASP 114 -8.205 37.586 50.600 1.000 30.79 114 3503 2856 5340 1229 1240 9 9 6 114 -7.242 36.402 50.648 1.000 26.16 ANISOU 756 C ATOM 757 O ASP 114 2581 2404 4955 601 1114 8 0 4 114 -6.031 36.458 50.338 1.000 25.45 ASP ANISOU 757 O ASP 114 2302 2503 4866 -43 602 131 ATOM 758 CB ASP 114 -8.595 37.874 52.075 1.000 43.68 ANISOU 758 CB ASP 114 7509 2783 6304 1157 2727 - 210 ATOM 114 -7.391 38.386 52.835 1.000 46.96 759 CG ASP ANISOU 759 CG ASP 114 9259 3225 5359 2517 519 107 ATOM 760 OD1 ASP 114 -6.487 38.959 52.189 1.000 83.49 ANISOU 760 OD1 ASP 114 13724 9866 8132 -6354 650 -3056 761 MOTA OD2 ASP 114 -7.370 38.262 54.071 1.000113.59 ANISOU 761 OD2 ASP 114 27880 10550 4730 -6984 -159 -2575 ATOM 762 N PHE 115 -7.831 35.323 51.153 1.000 22.32 ANISOU 762 N PHE 115 2620 2062 3799 204 954 - 114 ATOM 763 CA PHE 115 -7.115 34.026 51.183 1.000 22.69

- 38 -ANISOU 763 CA PHE 115 2765 1909 3947 118 1093 - 187 764 С PHE 115 -6.502 33.754 49.816 1.000 21.49 ANISOU 764 C PHE 115 2146 2316 3702 305 559 - 255 MOTA 765 0 PHE 115 -5.328 33.362 49.758 1.000 20.51 ANISOU 765 0 PHE 115 2153 3627 2011 323 488 -158 ATOM 766 CВ 115 -8.096 PHE 32.928 51.638 1.000 20.76 ANISOU 766 CB PHE 115 2369 1946 3574 -3 563 -473 MOTA 767 CG 115 -7.496 31.590 PHE 51.998 1.000 20.23 ANISOU 767 CG PHE 115 2369 1854 -155 629 -377 3463 768 CD1 PHE 115 -6.915 30.756 51.041 1.000 20.35 ANISOU 768 CD1 PHE 115 2572 1786 3372 -195 112 -756 ATOM 769 CD2 PHE 115 -7.474 31.152 53.309 1.000 21.11 ANISOU 769 CD2 PHE 115 2802 1932 3287 -113 17 - 689 MOTA 770 CE1 PHE 115 -6.351 29.538 51.325 1.000 21.09 ANISOU 770 CE1 PHE 115 2502 3784 1728 -295 471 -538 ATOM 771 CE2 PHE 115 -6.938 29.901 53.623 1.000 27.40 ANISOU 771 CE2 PHE 115 5012 1955 ذ443 444 43 - 572 MOTA 772 CZ PHE 115 -6.332 29.110 52.655 1.000 24.92 ANISOU 772 CZPHE 115 3356 1889 4222 50 1519 221 773 ATOM Ν GLU 116 -7.301 33.768 48.757 1.000 21.64 ANISOU 773 N GLU 116 2396 1835 3990 338 261 - 13 ATOM 774 CA GLU 116 -6.750 33.424 47.444 1.000 20.90 ANISOU 774 CA GLU 116 2235 1965 3742 224 74 1 1 6 ATOM 775 C GLU 116 -5.550 34.262 47.054 1.000 20.32 ANISOU 775 С GLU 116 1978 1899 3845 439 -108 4 4 8 ATOM 776 0 GLU 116 -4.544 33.679 46.604 1.000 20.18 ANISOU 776 0 GLU 116 2209 2147 3312 424 73 1 3 9 ATOM 777 СВ 116 -7.851 33.561 116 2425 2638 GLU 46.385 1.000 24.22 ANISOU 777 CВ GLU 2638 -.467 -237 5 1 9 4139 MOTA 778 CG GLU 116 -7.339 33.331 44.980 1.000 23.27 3952 -7 -494 750 ANISOU 778 116 2425 CG GLU 2465 ATOM 779 CD GLU 116 -8.401 33.273 43.910 1.000 25.02 ANISOU 779 CD GLU 116 2695 2703 4107 -510 -739 1509 MOTA 780 116 -9.617 33.306 OE1 GLU 44.207 1.000 34.83 ANISOU 780 OE1 GLU 116 2466 4606 6161 -203 -928 1566 MOTA 781 OE2 GLU 116 -8.001 33.030 42.763 1.000 40.92 ANISOU 781 OE2 GLU 116 4389 7172 3988 -24 -968 6 9 3 ATOM 782 Ν ARG 117 -5.549 35.571 47.300 1.000 20.60 ANISOU 782 Ν ARG 117 2299 1811 3718 382 -10 469 ATOM 783 CAARG 117 -4.374 36.374 46.866 1.000 22.65 ANISOU 783 CA117 2230 ARG 1791 4586 351 107 153 ATOM 784 С 117 -3.163 35.911 47.648 1.000 21.87 ARG ANISOU 784 С ARG 117 2269 1865 4178 252 179 9 7 ATOM 785 0 ARG 117 -2.060 35.789 47.102 1.000 22.10 ANISOU 785 0 ARG 117 2197 2270 3931 216 41 2 0 5 ATOM 786 CB ARG 117 -4.682 37.861 47.105 1.000 29.47 ANISOU 786 CB ARG 117 2849 1691 6658 259 -555 - 1 ATOM 787 CG 117 -3.485 ARG 38.815 47.046 1.000 40.24 ANISOU 787 CG ARG 117 3905 2567 8818 -819 -1330 -476 ATOM 788 CD ARG 117 -3.745 40.160 47.716 1.000 52.75 ANISOU 788 CD ARG 117 4698 2848 12496 -595 -1653 ATOM 789 NΕ 117 -3.934 ARG 39.987 49.155 1.000 68.00 ANISOU 789 NΕ ARG 117 8247 4719 12872 422 1842 - 3441 ATOM 790 CZARG 117 -3.166 40.448 50.126 1.000 78.38

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49.849 1.000 89.01

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11947 2617 2551 - 2095

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117 13026

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117 14218

117 -3.479

118 -3.334

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NH2 ARG

NH2 ARG

- 39 -794 CA ILE 118 -2.206 35.425 49.810 1:000 20.99 ANISOU 794 118 2546 1624 3 8 0 5 408 294 - 470 MOTA 795 ILE 118 -1.596 34.073 49.475 1.000 18.79 ANISOU 795 C ILE 118 2222 15343384 218 573 - 201 ATOM 796 0 ILE 118 -0.409 33.858 49.323 1.000 17.27 ANISOU 796 0 ILE 118 2194 1663 2707 283 351 - 136 797 CB ILE 35.542 118 -2.588 51.293 1.000 22.62 ANISOU 797 CB ILE 118 2702 1997 3895 276 416 -856 798 ATOM CG1 ILE 51.700 1.000 27.54 118 -2.916 36.995 ANISOU 798 CG1 ILE 118 5077 1801 3587 503 768 ATOM 799 118 -1.552 34.940 CG2 ILE 52.206 1.000 23.59 ANISOU 799 CG2 ILE 118 3084 2274 3606 183 254 ATOM 800 CD1 ILE 118 -3.493 37.115 53.096 1.000 29.35 ANISOU 800 CD1 ILE 118 5212 2054 3885 558 1114 - 645 MOTA 801 N TRP 119 -2.454 33.069 49.341 1.000 17.93 ANISOU 801 TRP 119 2378 1605 119 -2.035 31.688 Ν 2828 147 -80 - 2.69 CA TRP ATOM 802 49.103 1.000 16.57 ANISOU 802 CA TRP -25 - 16 TRP ATOM 803 C ANISOU 803 C 119 2126 TRP 1723 2604 269 -91 -51 119 -0.700 30.640 47.455 1.000 17.58 MOTE804 0 TRP ANISOU 804 0 TRP 119 1892 1674 3113 135 181 6 3 119 -3.127 30.690 49.591 1.000 18.32 MOTA 805 CB TRP ANISOU 805 CB TRP 119 2156 1789 3014 -34 5 -MOTA 805 CG TRP 119 -2.934 30.457 51.082 1.000 18.27 ANISOU 806 CG TRP 119 2208 1711 - 3025 86 349 5 6 MOTA 807 CD1 TRP 119 -3.354 31.273 52.103 1.000 20.36 119 2624 - 2029 3083 156 270 - 119 -2.213 29.383 51.683 1.000 18.61 2055 2967 134 263 1 ANISOU 807 CD1 TRP 276 - 153 ATOM 808 CD2 TRP ANISOU 808 CD2 TRP 263 110 119 -2.955 30.773 53.323 1.000 20.55 ATOM 809 NE1 TRP NE1 TRP ANISOU 809 119 2471 2229 3109 92 266 - 106 MOTA 810 119 -2.260 29.603 CE2 TRP 53.073 1.000 20.21 ANISOU 810 CE2 TRP 119 2529 2258 2893 180 754 297 MOTA 811 119 -1.576 28.258 51.147 1.000 18.29 CE3 TRP ANISOU 811 CE3 TRP 119 2258 1714 2977 42 -70 - 20 ATOM 812 CZ2 TRP 119 -1.636 28.728 53.981 1.000 21.97 CZ2 TRP ANISOU 812 1-19 2876 2526 2945 384 51 - 106 ATOM 813 119 -0.968 27.375 52.045 1.000 19.35 CZ3 TRP ANISOU 813 CZ3 TRP 119 2576 2028 2750 187 415 299 ATOM 814 CH2 TRP 119 -1.026 27.618 53.442 1.000 21.67 ANISOU 814 CH2 TRP 250 9 7 ATOM 815 THR N ANISOU 815 N THR 2577 122 -112 1 8 CA THR ATOM 816 ANISOU 816 CA THR 120 1915 2469 2398 222 -371 - 3 2 4 MOTA 817 C THR 120 2031 1855 2629 241 -155 1 120 0.700 31.960 44.674 1.000 18.67 ANISOU 817 C THR 2629 241 -155 1 9 2 ATOM 818 0 THR ANISOU 818 0 THR 120 1996 1887 3212 389 -131 1 7 7 MOTA 819 CB THR 120 -2.487 32.865 44.344 1.000 18.10 ANISOU 819 CB THR 120 1951 2204 2720 28 -93 3 4 5 MOTA 820 OG1 THR 120 -3.773 32.238 44.284 1.000 20.49 ANISOU 820 OG1 THR 120 1807 2801 3179 59 - 363 558 MOTA 821 CG2 THR 120 -1.919 32.803 42.933 1.000 22.46 ANISOU 821 CG2 THR 120 2438 3266 2830 118 705 475 MOTA 822 N GLN 121 0.094 33.708 45.956 1.000 18.62 ANISOU 822 Ν GLN 121 2180 1657 3237 -94 213 123 823 CA GLN 121 1.466 121 2077 34.232 45.993 1:000 18.15 ANISOU 823 CA GLN 1698 3119 77 96 5 2 0 MOTA 824 GLN 121 2.412 33.284 46.718 1.000 17.04

						- 40 -			
ANISOU		С	GLN	121	2022	1431	3019	192	234 223
ATOM	825	0	GLN		3.510	33.047	46.270		19.32
ANISOU		0	GLN		1894	1800	3645		6 1 2 9
ATOM	826	СB	$\operatorname{GLN}$	121		35.579	46.756	1 000	22.90
ANISOU		СВ	GLN	121		1479	4702	327	-812 2 7 1
ATOM	827	CG	GLN	121	2.888	36.159	46.871	1 000	27.04
ANISOU		CG	GLN	121		2062	5262	-346	-400 1 3 2
ATOM	828	CD	GLN	121	3.530	36.511		1 000	31.94
ANISOU		CD	GLN	121	3307	2733	6097	983	1031 9 9
ATOM	829		GLN	121	4.660	36.085	45.247	1 000	62.76
ANISOU			GLN	121	3009	9570	11267	1758	2366 2029
ATOM	830		GLN	121	2.859	37.306	44.716		55.89
ANISOU			GLN	121		7728	6993	2815	1745 3249
ATOM	831	N	TYR	122		32.791		1.000	16.87
ANISOU		N	TYR	122	2389	1518	2501	71 -1	61 - 54
ATOM	832	CA	TYR	122		31.881	48.683	1.000	17.97
ANISOU ATOM	833	CA	TYR	122	2564	1600	2666	176	-224 - 56
ANISOU		C	TYR	122	3.080	30.600	47.909	1.000	16.83
ATOM	834	C 0	TYR		1870	1460	3065	-31	-57 - 98
ANISOU		0	$ ext{TYR}$	122		30.129	47.823	1.000	17.67
ATOM	835	СВ	TYR	122	1891	1952	2872	189	-220 1 2 6
ANISOU		CB	TYR	122	2.018 2526	31.522	49.960		18.01
ATOM	836	CG	TYR		2.753	1821	2495	2 -3	
ANISOU		CG	TYR	122	2332	30.619 1695	50.898		17.89
ATOM	837		TYR		4.058	30.901	2769	255	-147 - 51 21.71
ANISOU	837		TYR	122	2883	2101	3267	-257	
ATOM	838	CD2	TYR	122:	2.107	29.496	51.415		-913 3 4
ANISOU			TYR	122	2428	2026	3634	128	-267 4 6 8
ATOM	839	CE1	TYR	122	4.680	30.037	52.212	1.000	21 27
ANISOU ATOM			TYR	122	2681	2045	3356	140	-725 - 210
ANISOU	840	CEZ	TYR	122	2.746	28.637	52.290	1.000	24.50
ATOM	841	CZ	TYR TYR	122	3376	1876	4057 -	-292	-1163 506
ANISOU	841	CZ	TYR	122	4.043 3161	28.914	52.675	1.000	22.16
ATOM	842	OH	TYR		4.699	1881	3379	95 -90	09 -128
ANISOU		OH	TYR		3471	28.079 2398	53.566	1.000	23.72
ATOM	843	N	PHE		2.074	30.023	3142	52 -10	005 - 56
ANISOU	843	N	PHE		1794	1571	47.253 2793		
ATOM	844	CA	PHE	123	2.347	28.843	46.397	1 000	5 - 5 4
ANISOU	844	CA	PHE	123	1622	1800	2548	34 -14	
ATOM	845	С	PHE	123	3.378	29.188	45.337	1 000	15 96
ANISOU		C	PHE		1681	1304	3078	42 90	3
ATOM ANISOU	846	0	PHE	123	4.276	28.375	45.037	1.000	15.47
ATOM	847	0	PHE	123	1703	1437	2739	54 14	- 2 4
ANISOU		CB CB	PHE PHE		1.036	28.309	45.779	1.000	15.07
ATOM	848	CG	PHE	123	1460	1364	2904	209	-148 1
ANISOU.	848	CG	PHE	123	1.24 2090	27.104	44.879	1.000	
ATOM	849		PHE	123	1.170	1620	2906	-39	-179 -238
ANISOU	849	CD1	PHE	123	1680	25.831 1439	45.452	1.000	17.41
ATOM	850	CD2	PHE	123	1.490	27.259	3434 ·	12 -11	L9 - 255
ANISOU	850	CD2	PHE	123	1723	2331	43.513 2870	-96	
ATOM	851	CE1	PHE		1.419	24.740	44.636		-216 - 372
ANISOU		CE1	PHE	123	2112	1766	3397	212	-540 - 536
ATOM	852	CE2	PHE	123	1.722	26.144	42.717		19.63
ANISOU ATOM		CE2			1901	2476	3083	-134	-261 -632
ANISOU	853 853	CZ CZ	PHE		1.635	24.868	43.274	1.000	19.40
ATOM	854	N N	PHE ASP		1525	2424	3421	385	-529 -490
ANISOU	854	N	ASP		3.164 1947	30.304		1.000	
	1	••		124	174/	1466	2992	-23	-110 1 2 4

- 41 -CA ASP 124 4.060 CA ASP 124 2103 855 ATOM 30.640 43.544 1.000 17.82 ANISOU 855 124 2103 405 -24 314 ATOM 856 С ASP С ANISOU 856 ASP 124 1999 1439 3219 181 MOTA 857 0 ASP 124 6.402 30.324 43.317 1.000 17.18 ANISOU 857 0 ASP 124 2086 1427 3015 34 181 1 7 7 AASP 124 3.639 ATOM 858 CЭ 31.997 42.942 0.534 21.77 AASP 124 3475 ANISOU 858 CВ 2089 2706 -372 5 9 7 642 32.30 1982 1 538 AASP 124 4.381 859 CG 32.304 41.659 0.534 19.28 ANISOU 859 CG AASP 124 2376 2967 173 -553 4 9 5 MOTA 860 OD1 AASP 124 4.223 31.538 40.678 0.534 21.03 ANISOU 860 OD1 AASP 124 2189 2636 76 2 1 3164 -28 OD2 AASP 124 5.068 33.348 41.639 0.534 24.96 ATOM 861 ANISOU 861 OD2 AASP 124 3681 2052 3752 -296 -1067 889 CB BASP 124 3.632 31.975 42.908 0.466 19.67 ATOM 862 BASP 124 2559 1993 2923 1003 673 4 ABASP 124 2.368 31.849 42.089 0.466 22.78 ANISOU 862 СЗ 1003 673 446 MOTA 863 CG CG BASP 124 2.368 31.849 42.089 0.466 22.78
CG BASP 124 3552 3217 1889 872 177 1175
OD1 BASP 124 2.021 30.781 41.545 0.466 27.78
OD1 BASP 124 2138 3932 4483 100 503 3 4 7
OD2 BASP 124 1.703 32.893 41.902 0.466 29.73
OD2 BASP 124 3845 3804 3646 1239 -312 1644
N ARG 125 5.669 31.416 45.153 1.000 16.65
N ARG 125 1942 1350 3032 276 139 2 7 6 ANISOU 863 872 1.77 1175 ATOM 864 ANISOU 864 865 ANISOU 865 3646 1239 -312 1644 MOTA 866 ANISOU 866 N ARG 125 1942 1350 3032 276 139 276 CA ARG 125 7.038 31.528 45.646 1.000 17.58 ATOM 867 ANISOU 867 CA ARG 125 1918 1819 2944 98 177 2 4 1 C ARG 125 7.662 30.188 45.992 1.000 17.38 MOTA 868 C ARG 125 1544 1777 3282 -42 40 27: O ARG 125 8.841 29.942 45.754 1.000 18.26 ANISOU 868 3282 -42 40 273 ATOM 869 125 1639 1669 3631 -97 91 -233 125 7.062 32.468 46.851-1.000 20.45 125 2219 2162 3387 -244 450 -274 125 6.860 33.916 46.344 1.000 28.23 O ARG CB ARG ANISOU 869 ATOM 870 CB ARG ANISOU 870 2007 34.80 ATOM 871 ARG CG ANISOU 871 CG ARG ATOM 872 CD 125 6.693 34.891 47.477 1.000 31.76 ARG ANISOU 872 CD ARG 125 3065 6725 -628 1455 -993 2279 125 6.496 36.221 125 3332 2095 ATOM 873 NΞ ARG 36.221 46.932 1.000 40.81 ANISOU 873 NE ARG 10080 -169 1790 -694 125 5.970 37.229 47.628 1.000 43.42 ATOM 874 CZ ARG ANISOU 874 CZ ARG 125 4531 2891 9076 839 2072 - 188 125 5.551 37.025 48.866 1.000 38.62 125 3999 2858 7816 -858 61 -700 ATOM 875 NH1 ARG ANISOU 875 NH1 ARG ATOM NH2 ARG 125 5.858 38.382 47.006 1.000 42.11 876 ANISOU 876 
 125
 5319
 2652
 8030
 908
 1627

 126
 6.884
 29.282
 46.557
 1.000
 15.28
 NH2 ARG 1627 - 681 ATOM 877 N GLN 
 126
 6.884
 29.282
 46.55/1.000
 15.28

 126
 1876
 1527
 2404
 -70
 13 - 60

 126
 7.376
 27.929
 46.853
 1.000
 15.37

 126
 1726
 1625
 2488
 -54
 -312
 20

 126
 7.649
 27.150
 45.578
 1.000
 14.21

 126
 1643
 1268
 2488
 -75
 -398
 7

 126
 8.682
 26.462
 45.496
 1.000
 15.36

 126
 1531
 1554
 2753
 -37
 -316
 5

 126
 6.356
 27.158
 47.702
 1.000
 17.40

 126
 2034
 1313
 3264
 158
 293
 4
 N ANISOU 877 GLN CA GLN ATOM 878 ANISOU 878 CA GLN GLN MOTA 879 C ANISOU 879 C GLN ATOM 880 O GLN ANISOU 880 O GLN ATOM CB GLN 881 ANISOU 881 CB GLN 
 126
 2034
 1313
 3264
 158
 293
 4

 126
 6.336
 27.634
 49.150
 1.000
 26.14
 3264 158 293 4 3 MOTA 882 CG GLN ANISOU 882 CGGLN 126 4503 1690 3739 431 1908 - 732 ATOM 883 CD GLN 126 5.208 26.998 49.891 1.000 21.95 ANISOU 883 CDGLN 126 2957 2670 2713 0 -123 1 0 2 ATOM 884 OE1 GLN 126 4.051 27.372 49.730 1.000 42.52 ANISOU 884 OE1 GLN 126 2994 5747 7416 -62 -1272 3147 MOTA NE2 GLN 885 126 5.524 26.003 50.691 1.000 28.32

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- 42 -
 ANISOU 885
             NE2 GLN 126 2867
                                  3971
                                          3922
                                                 -184 -780 1311
        886
                 TYR
             N
                      127 6.797
                                  27.287
                                          44.574 1.000 14.52
 ANISOU 886
             Ν
                 TYR
                      127 1629
                                  1438
                                          2448
                                                 -41
                                                     -373 - 36
 ATOM
        887
             CA
                 TYR
                      127 7.039
                                  26.554
                                          43.317 1.000 13.93
 ANISOU 887
             CA
                      127 1563
                 TYR
                                  1455
                                          2277
                                                 -136
                                                      -234 1 5 0
 ATOM
        888
             C
                 TYR
                      127 8.289
                                  27.091
                                          42.624 1.000 14.54
 ANISOU 888
             C
                      127 1461
                 TYR
                                  1318
                                          2745
                                                24 -195 190
 MOTA
        889
             0
                 TYR
                      127 9.133
                                  26.345
                                          42.140 1.000 14.39
                      127 1611
127 5.801
127 1510
 ANISOU 889
             0
                 TYR
                                 1580
                                          2277
                                                34 -252 9
 ATOM
        890
                TYR
            СB
                                 26.676
                                         42.435 1.000 14.00
 ANISOU 890
            CB TYR
                                 1549
25.795
                                          2258
                                                29 -180 - 70
 ATOM
        891
                      127 5.752
             CG
                TYR
                                         41.202 1.000 12.33
 ANISOU 891
             CG TYR
                      127 1315
                                 1037
                                         2334
                                              -34 -187 4 5
 ATOM
        892
             CD1 TYR
                     127 6.483
                                 24.626
                                         41.024 1.000 14.05
 ANISOU 892
             CD1 TYR
                     127 1810
                                 1158
                                         2371 7 -84 - 8
 ATOM
        893
             CD2 TYR
                                26.086 40.206 1.000 15.71
                     127 4.837
 ANISOU 893
             CD2 TYR
                     127 1936
                                 1548
                                         2484
                                                55 -513 2 1
 ATOM
        894
             CE1 TYR
                     127 6.382
                                23.829 39.899 1.000 13.10
 ANISOU 894
             CE1 TYR
                     127 1450
                                 999 2529 -101 -227 -62
ATOM
        895
             CE2 TYR
                     127 4.661
                                25.322 39.071 1.000 15.07
ANISOU 895
             CE2 TYR
                     127 1928
127 5.440
                                 1620
                                         2177
                                                158 - 342 1 9 7
ATOM
       896
             CZ TYR
                                24.179
                                         38.934 1.000 13.71
ANISOU 896
             CZ
                TYR
                     127 1617
                                 1348
                                         2245
                                                -146 -106 2 4 6
MOTA
       897
                     127 5.337
             ОН
               TYR
                                 23.386
                                         37.811 1.000 15.04
ANISOU 897
             OH TYR
                     127 1682
                                 1755
                                         2279
                                                -87
                                                     -60 5 3
ATOM
       898
            N
                THR
                     128 8.467
                                 28.412
                                         42.616 1.000 14.69
ANISOU 898
            N
                THR
                     128 1813
                                 1324
                                         2446
                                                -154 -217 2 6 8
ATOM
       899
            CA THR
                     128 9.673
                                 28.984
                                         42.011 1.000 14.67
-ANISOU 899
            CA THR
                     128 1867
                                 1469
                                         2238
                                                     -32 195
                                                -98
MOTA
       900
            C
                THR
                     128 10.921 28.552
                                         42.736 1.000 14.68
ANISOU 900
            C
                THR
                     128 1794
                                 1318
                                         2466
                                              59 -123 -285
ATOM
       901
                     128 11.900 28.166 42.062 1.000 15.45
            0
                THR
ANISOU 901
            0
                THR
                     128 1715
                                1487
                                         2667
                                                -259 153 7
ATOM
       902
            CB THR
                     128 9.572
                                30.544 42.069 1.000 16.02
ANISOU 902
            CB THR
                     128 2043
                                 1348
                                         2695
                                               -79
                                                      59 4 7 9
ATOM
       903
            OG1 THR
                     128 8.519
                                 30.849 41.162 1.000 19.14
ANISOU 903
            OG1 THR
                     128 2226
                                 2038
                                         3008
                                                195 -23 545
ATOM
                     128 10.835 31.187 41.582 1.000 19.03
       904
            CG2 THR
ANISOU 904
            CG2 THR
                     128 2107
                                 1329
                                         3793
                                                125
                                                      311 618
MOTA
                    129 10.933 28.564 44.085 1.000 14.21
       905
            Ν
              ALA
ANISOU 905
            N
                ALA
                    129 1708
                                 1266
                                         2424
                                                -137 -256 -181
ATOM
       906
            CA ALA
CA ALA
                    129 12.108 28.110 44.836 1.000 15.08
ANISOU 906
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                                 1435
                                         2624
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MOTA
       907
            С
                ALA
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ANISOU 907
            С
                ALA
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ATOM
       908
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                     129 13.552
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ANISOU 908
            0
                ALA
                     129 1758
                                 1464
                                         2137
                                                -5 -244 -148
ATOM
       909
            CВ
               ALA
                    129 11.887
                                 28.313 46.313 1.000 17.08
ANISOU 909
            СВ
               ALA
                    129 2132
                                 1851
                                         2506
                                                -183 -514 -239
ATOM
       910
            N
                SER
                    130 11.343
                                 25.819
                                        44.553 1.000 14.18
ANISOU 910
            N
                SER
                    130 1884
                                 1237
                                         2267
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ATOM
       911
            CA
               SER
                    130 11.487
                                 24.375
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ANISOU 911
            CA SER
                    130 1840
                                 1219
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ATOM
       912
            С
                SER
                    130 12.072
                                 24.114
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ANISOU 912
            С
                SER
                    130 1345
                                 1481 2665 78 -796 - 209
23.329 42.807 1.000 14.43
                                 1481
                                         2665
ATOM
       913
            0
                SER
                    130 13.037
ANISOU 913
            0
                SER
                     130 1327
                                 1382
                                         2773
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                                                     -246 172
       914
MOTA
            СВ
               SER
                     130 10.120
                                 23.677 44.663 1.000 17.54
ANISOU 914
            СВ
                SER
                     130 1555
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ATOM
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            OG
                SER
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ANISOU 915
            OG
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- 43 -ARG 131 11.555 24.772 41.909 1.000 14.47
ARG 131 1421 1448 2628 161 -384 - 1
ARG 131 12.163 24.598 40.592 1.000 14.91
ARG 131 1689 1452 2525 -4 -526 - 34 916 N ANISOU 916 N-384 **-**166 CA ARG ATOM 917 ANISOU 917 131 1689 1452 2525 -4 -526 -341 131 13.605 25.079 40.566 1.000 14.05 ATOM 918 C ARG 131 1772 ANISCU 918 С ARG 1435 2132 -72 -381 - 173 24.438 39.912 1.000 15.14 ATOM 919 0 ARG 131 14.448 ANISOU 919 0 ARG 131 1829 1658 2267 -109 -170 - 230 131 11.349 25.316 39.514 1.000 15.77 920 CB ARG ANISOU 920 CB ARG 131 1720 1613 2660 -54 -493 - 94 ATOM 921 CG ARG 131 9.70 24.737 39.251 1.000 16.08

ANISOU 921 CG ARG 131 1703 1695 2711 -13 -647 - 141

ATOM 922 CD ARG 131 9.326 25.390 38.017 1.000 26.56

ANISOU 922 CD ARG 131 3589 2689 3813 -1037 -2156 7 4 5

ATOM 923 NE ARG 131 9.327 26.831 37.918 1.000 25.91

ATOM 924 CZ ARG 131 8.472 27.716 38.413 1.000 31.86

ANISOU 924 CZ ARG 131 8.472 27.716 38.413 1.000 31.86

ANISOU 924 CZ ARG 131 8.472 27.724 39.138 1.000 31.34

ANISOU 925 NH1 ARG 131 7.467 27.244 39.138 1.000 31.34

ANISOU 926 NH2 ARG 131 8.633 29.032 38.235 1.000 40.12

ANISOU 926 NH2 ARG 131 8.633 29.032 38.235 1.000 40.12

ANISOU 927 N ALA 132 13.893 26.186 41.236 1.000 13.42

ANISOU 927 N ALA 132 1683 1385 20.33 -85 -652 - 2 4

ANISOU 928 CA ALA 132 1617 1443 20.22 -16 -499 - 7 9

ATOM 929 C ALA 132 16.225 25.808 41.837 1.000 13.37

ANISOU 929 C ALA 132 16.225 25.808 41.837 1.000 13.37

ANISOU 929 C ALA 132 16.225 25.808 41.837 1.000 13.37

ANISOU 929 C ALA 132 16.225 25.808 41.837 1.000 13.37

ANISOU 929 C ALA 132 15.246 25.586 41.328 1.000 14.43

ANISOU 930 O ALA 132 1459 1772 2251 -91 -240 1 0 6

ATOM 931 CB ALA 132 15.275 28.084 41.859 1.000 16.52

ANISOU 931 CB ALA 132 15.893 25.248 42.996 1.000 13.62 CG ARG 131 9.970 24.737 39.251 1.000 15.08 921 ATOM 132 1459 1772 2251 -91 -240 1 0 6 132 15.275 28.084 41.859 1.000 16.52 132 2019 1243 3014 -199 -366 -2 3 6 133 15.893 25.248 42.996 1.000 13.62 932 N VAL ATOM ANISOU 932 N VAL 133 1522 1515 2139 -63 -362 8 6 133 16.839 24.363 43.689 1.000 14.86 133 1902 1566 2179 120 -491 - 27 133 1522 936 CB VAL 133 1528 1789 2234 -45 -391 2 1 0
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938 CG2 VAL 133 1769 1942 2561 -61 -831 6 4
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ANISOU 1060 O
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                    150 12.531 24.305
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               GLU
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ANISOU 1061 CB
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ANISOU 1063 CD
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MOTA
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ANISOU 1064 OE1 GLU
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                                         3648
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       1065 OE2 GLU
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ANISOU 1065 OE2 GLU
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MOTA
       1066 N
                ALA
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ANISOU 1066 N
                ALA
                     151 1649
                                1710
                                         2334
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       1067 CA
MOTA
                ALA
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ANISOU 1067 CA
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ATOM
       1068 C
                ALA
                     151 9.748
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                                         31.724 1.000 15.38
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						- 48 -				
ANISOU			ALA	151	1674	1953	2216	165	181 44	2
ATOM	1069	9 0	ALA	151	8.642	19.136	32.184	1 000	16.51	ے
ANISOU			ALA	151		1852	2643	-152	110 33	$\cap$
ATOM	1070		ALA	151	9.823	19.663	29.236		18.05	U
ANISOU			ALA	151	1910	2811	2139	-275	-316 1 6	_
ATOM	1071	N	PHE	152	10.893	19.135		1 000	14.25	0
ANISOU			PHE	152		1132				
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ANISOU			PHE	152	1457	1291	2353	1000		
ATOM	1073		PHE	152		19.056	34.695	1 000		Ŧ
ANISOU			PHE		1481		2412	-43		_
ATOM	1074	. 0	PHE		9.679	18.495	35 552	1 000	-165 1 9 6 14.50	)
ANISOU	1074	. 0	PHE	152		1482	2438	-85	25 2 6	
ATOM	1075		PHE	152	12.309	17.744		1 000	13.95	
ANISOU	1075	CB	PHE	152		1547	2248	-29		,
$\mathtt{ATOM}$	1076		PHE	152	12.475	16.966		1 000	111 463 14.04	)
ANISOU		CG	PHE	.152	1747	1386	2200	88 -5	8 2 4 7	
MOTA	1077	CD1	PHE	152	12.032	15.653		1 000	13.90	
ANISOU	1077	CD1	PHE	152	1906	1306	2069	165	-36 281	
ATOM	1078	CD2	PHE	152	13.094	17.499		1 000	15.67	_
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ANISOU	1079	CE1	PHE	152	1669	1507	2165	182	-282 3 4 7	7
ATOM	1080	CE2	PHE	152	13.323	16.799	37.276	1.000	14 83	'
ANISOU	1080	CE2		152	1724	1671 -	2240	35 -1	12 165	
ATOM	1081		PHE	152	12.861	15.522	37.361	1.000	14.86	
ANISOU	1081		PHE	152	1994 -	1734	1916	-162	99 1 1 3	
ATOM	1082		LEU	153	10.789	20.324	34.789	1.000	15.25	
ANISOU ATOM	1082		LEU	153	1742	1355	2696	58 11	0 1 5 4	
	1083		LEU	153	10.454	21.151	35.939	1.000	14.65	
ATOM	1083 1084	CA	LEU	153	1783	1429	2354	-66	16 2 0 3	
ANISOU	1084		LEU	153	9.082	21.791	35.877	1.000	14.47	
ATOM	1085		LEU	153	1732	1402	2362	-80	76 1 1	
	1085		LEU		8.581	22.216	36.953	1.000	15.82	
ATOM	1085	C D	LEU		1940	1454	2616	-313	312 - 15	7
	1086		LEU LEU	153	11.537	22.224	36.165		16.53	
ATOM	1087		LEU		1626	1451	3205	-23	269 - 83	,
ANISOU	1087	CG	LEU	153	12.914 1893	21.685	36.514			
ATOM	1088		TEU	153	13.922	2013	2135	-33	-186 - 36	,
ANISOU	1088	CDI	T.FIT			22.829	36.614	1.000	18.41	
ATOM	1089	CD2	LFII		1732 12.863	2473	2791	-156	80 - 876	
ANISOU	1089	CD2	LEU	153	3083	20.883 3182	37.794			
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ANISOU	1090	N	ASP		1768	1181	2525		14.41	
ATOM	1091	CA	ASP	154	7.092	22.373		-25	-8 2 9 3	
ANISOU	1091	CA	ASP	154	1665	1615	34.553			
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ANISOU	1092	С	ASP	154	1859	1304	34.814 2409			
ATOM	1093		ASP	154	5.995	20.368	33.889	-92	143 515	,
ANISOU	1093		ASP	154	2561	1455	2557	-29		
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ANISOU	1094	СВ	ASP	154	1905	2077	3081	124		7
ATOM	1095	CG	ASP	154	5.461	23.157	32.768	1 000	269 131	/
	1095	CG	ASP	154	2029	2531	2990	226		6
ATOM	1096	OD1	ASP	154	4.561	23.253	33.639		129 143 19.68	O
ANISOU	1096	OD1	ASP	154	1949	2209	3318	92 221		
ATOM	1097	OD2	ASP	154	5.207	23.189	31.554	1 000	) 7 <i>7</i> 7	
ANISOU	1097	OD2	ASP	154	2512	3475	3029	246	-137 6 5 3	
ATOM	1098	N	CYS	155	5.831	20.904	36.070		14 25	,
ANISOU	1098	N	CYS	155	1708	1365	2342	-101	-62 546	
								<b>1</b> 0 1	-04 0 4 0	;

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- 49 -155 5.418 155 1608 ATOM 1099 CA CYS 19.569 36.468 1.000 13.45 1346 ANISOU 1099 CA CYS 2158 -191 4 458 155 4.157 1346 2158 -191 4 4 5 8 19.574 37.302 1.000 12.49 ATOM 1100 C CYS 155 1644 ANISOU 1100 C CYS 1331 1772 -200 -148 6 2 36.941 1.000 14.55 ATOM 1101 0 CYS 155 3.224 20.303 ANISOU 1101 O 155 1633 CYS 1492 2402 -122 -111 4 4 2 18.872 37.098 1.000 14.37 ATOM 1102 CB CYS 155 6.664 ANISOU 1102 CB CYS 155 1907 1366 2186 122 -137 2 1 1 19.595 38.641 1.000 14.99 ATOM 1103 SG CYS 155 7.265 ANISOU 1103 SG CYS 155 1561 1821 2315 -74 -98 182 MOTA 1104 N GLU 156 4.060 18.706 38.316 1.000 12.89 ANISOU 1104 N GLU 156 1575 1379 1945 -130 29 1 9 4 ATOM 1105 CA GLU 156 2.788 18.447 39.029 1.000 12.98 ANISOU 1105 CA GLU 156 1508 1311 2114 -210 21 140 ATOM 1106 C GLU 156 2.987 18.676 40.510 1.000 12.34 ANISOU 1106 C 156 1414 156 2.828 CLU 1198 2078 102 ATOM 1107 0 GLU 17.757 41.289 1.000 14.89 156 1875 156 2.278 ANISOU 1107 O GLU 1425 2359 -15 -54 442 1103 CB ATOM GLU 17.047 38.678 1.000 14.48 ANISOU 1108 CB GLU 156 1968 1323 2213 -279 120 8 7 156 1.855 17.038 37.227 1.000 14.86 1109 CG GLU ANISOU 1109 CG GLU 156 1894 1526 2227 -120 95 -152 MOTA 1110 CD 156 0.523 GLU 17.687 36.932 1.000 17.10 ANISOU 1110 CD GLU 156 2091 1976 2431 44 -4 144 156 -0.204 17.967 37.886 1.000 17.98 1111 OE1 GLU ANISOU 1111 OE1 GLU 156 1811 2155 2866 -35 10 - 355 ATOM 1112 OE2 GLU 17.990 35.759 1.000 20.99 156 0.214 150 0.214 1/.990 35.759 1.000 20.99 156 2854 2419 2704 -386 -516 5 6 2 157 3.292 19.893 40.958 1.000 12.09 157 1314 1347 1934 12 -48 2 4 9 157 3.576 20.121 42.391 1.000 13.28 157 1425 1696 1924 -68 117 1 4 7 157 2.330 19.996 43.248 1.000 12.87 157 1236 1737 1916 -214 -47 1 2 4 ANISOU 1112 OE2 GLU ATOM 1113 N PRO ANISOU 1113 N PRO 1114 CA PRO ATOM ANISOU 1114 CA PRO ATOM 1115 C PRO ANISOU 1115 C PRO 157 1.192 20.190 42.744 1.000 13.73 MOTA 1116 0 PRO ANISOU 1116 O PRO 157 1286 1717 2214 -190 -17 143 ATOM 1117 CB PRO 157 4.061 21.580 42.407 1.000 13.94 ANISOU 1117 CB PRO 157 1518 1729 2047 -289 -166 2 4 7 1118 CG ATOM PRO 157 3.363 22.184 41.226 1.000 13.06 ANISOU 1118 CG PRO 157 1558 1518 1887 -32 -158 - 88 1119 CD ATOM PRO 157 3.494 21.128 40.167 1.000 12.03 ANISOU 1119 CD 157 1521 158 2.542 PRO 1081 1968 -2 -7 1 2 1 1120 N ATOM LEU 19.738 44.526 1.000 13.02 ANISOU 1120 N LEU 158 1554 1493 1899 -124 148 7 3 ATOM 1121 CA 158 1.438 LEU 45.496 1.000 12.72 19.699 ANISOU 1121 CA LEU 158 1465 1552 1815 -126 -14 3 6 ATOM 1122 C 158 1.927 LEU 20.389 46.772 1.000 12.90 ANISOU 1122 C 158 1230 LEU 1715 1957 -27 -29 - 80 ATOM 1123 0 158 2.975 19.977 47.289 1.000 14.06 LEU ANISOU 1123 O LEU 158 1374 1666 2304 59 - 257 - 236 ATOM 1124 CB LEU 158 1.046 18.244 45.815 1.000 13.58 ANISOU 1124 CB LEU 158 1673 1590 1896 -213 57 1 7 1 MOTA 1125 CG LEU 158 0.044 18.030 46.945 1.000 14.84 ANISOU 1125 CG LEU 158 1471 2396 -16 262 242 1774 MOTA 1126 CD1 LEU 158 -1.333 18.635 46.671 1.000 16.96 ANISOU 1126 CD1 LEU 158 1485 2196 2764 5 -148 -401 ATOM 1127 CD2 LEU 158 -0.142 16.539 47.161 1.000 14.98 ANISOU 1127 CD2 LEU 158 1976 1820 1897 -390 171 7 9 ATOM 1128 N 159 1.139 LEU 21.306 47.283 1.000 13.44 159 1509 ANISOU 1128 N LEU 1434 2165 43 -87 -119 1434 2165 43 -8/-119 21.963 48.571 1.000 13.39 1129 CA LEU MOTA 159 1.443

- 50 -

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               LEU
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ANISOU 1139 O
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ANISOU 1146 NH2 ARG
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ANISOU 1147 N
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ANISOU 1148 CA PHE
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ANISOU 1298 CA THR 190 1292 1356 1903 -57 -221 -151
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ATOM
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ANISOU 1311 CD2 LEU 191 2297 1906 2837 -345 -437 1 48

ATOM 1312 N ILE 192 10.199 22.148 52.946 1.000 15.36
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ANISOU	J 1313	3 CA	ILE	192	1456	2043		1.000	
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ANISOU			ILE	192	1696	1973	22.010		15.58
ATOM	1315		ILE	192			2251	-199	
ANISOU	1315	5 0	ILE	192	1856	23.691	55.381		17.20
ATOM	1316		ILE	192		2449	2229	-307	-341 -574
ANISOU			ILE		9.722 2246	20.920	55.040	1.000	17.03
ATOM			ILE	100	9.454	1958	2266	-52	325 - 303
ANISOU	1317	CG1	TIE			19.596	54.317		19.80
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ANISOU	1319	CDI	TT E	192		18.387	55.235	1.000	31.57
ATOM	1320	· M	GLN		4558	2114	5222	-398	-1094 765
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	1327	OEI	GLN	193	7.193	28.695	53.688	1.000	45.31
ANISOU ATOM	1327	OEI	GLN	193	2826	7147	7241 🚄	-51	-616 3173
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- 57 *-*MOTA 1343 OG1 THR 26.550 195 4.111 63.196 1.000 25.45 ANISOU 1343 OG1 THR 195 3427 3101 3141 -9 -117 - 750 1344 CG2 THR MOTA 195 4.788 28.396 61.847 1.000 31.31 ANISOU 1344 CG2 THR 195 4965 2552 4380 274 -70 -409 MOTA 1345 N PRO 196 7.604 26.587 64.923 1.000 30.84 196 5225 ANISOU 1345 N PRO 3191 3300 785 -517 -1542 MOTA 1346 CA PRO 196 8.101 25.823 66.065 1.000 28.50 ANISOU 1346 CA PRO 196 3113 3700 4016 -279 -441 -646 MOTA 1347 C PRO 196 7.018 25.534 67.096 1.000 28.97 ANISOU 1347 C PRO 196 3581 3326 4102 42 113 -1381 MOTA 1348 0 PRO 196 6.002 26.229 67.192 1.000 32.32 ANISOU 1348 O PRO 196 4146 4649 3485 901 -180 -1658 1349 CB ATOM PRO 196 9.094 26.816 66.694 1.000 29.72 ANISOU 1349 CB PRO 196 3888 3292 4111 -285 -353 -1072 ATOM-1350 CG PRO 196 8.533 . 28.174 66.364 1.000 34.87 ANISOU 1350 CG PRO 196 6285 3575 3390 421 -1326 -1332 1351 CD MOTA PRO 196 7.897 28.035 65.012 1.000 33.20 ANISOU 1351 CD PRO 196 6407 3606 2600 -598 -494 -1031 197 7.289 ATOM 1352 N CYS 24.533 67.919 1.000 26.96 197 2739 ANISOU 1352 N CYS 4038 3465 -113 85 -1227 197 6.519 ATOM 1353 CA CYS 24.289 69.126 1.000 31.73 ANISOU 1353 CA CYS 197 3979 4543 3533 ~39 🗇 721 ATOM 1354 C CYS 197 6.803 25.412 70.124 1.000 35.58 ANISOU 1354 C CYS 197 4213 4819 4486 -480 1126 - 2282 ATOM 1355 0 197 7.917 CYS 25.939 70.175 1.000 31.34 ANISOU 1355 O CYS 197 3817 4845 3246 36 - 383 - 992 ATOM 1356 CB CYS 197 6.940 22.962 69.767 1.000 35.79 ANISOU 1356 CB 197: 5913 CYS 4705 2980 284 1566 - 1423 1357 SG - ATOM CYS 197 6.553 21.535 68.741 1.000 28.53 ANISOU 1357 SG CYS 197 3605 4224 3009 50 -5 - 452 ATOM 1358 N 198 5.771 ALA 25.791 70.866 1.000 37.27 ANISOU 1358 N 198 5038 ALA 4139 -421 1647 -2070 71.888 1.000 35.91 4984 1359 CA ALA MOTA 198 5.983 26.811 ANISOU 1359 CA ALA 198 6273 4144 3230 910 522 -1230 ATOM 1360 C ALA 198 6.993 26.-328 72.921 1.000 44.30 ANISOU 1360 C ALA 198 5998 6138 4696 -193 -199 3 3 1361 0 MOTA ALA198 7.759 27.127 73.457 1.000 42.85 ANISOU 1361 O ALA 198 5209 6328 4742 7 490 - 555 MOTA 1362 CB 198 4.671 ALA27.231 72.532 1.000 41.70 ANISOU 1362 CB ALA198 7588 5697 2557 2355 1068 - 721 ATOM 1363 N ASN 199 7.036 25.036 73.225 1.000 34.93 ANISOU 1363 N ASN 199 4027 5975 3270 805 167 -621 ATOM 1364 CA ASN 199 7.969 24.578 74.264 1.000 33.58 ANISOU 1364 CA ASN 199 3643 6167 2950 -670 -265 -808 ATOM 1365 C 199 9.352 ASN 24.262 73.718 1.000 31.53 ANISOU 1365 C ASN 199 4077 5048 2853 384 -420 -855 ATOM 1366 0 ASN 199 10.153 23.667 74.467 1.000 36.33 ANISOU 1366 O ASN 199 4223 5624 3957 -403 -1305 ATOM 1367 CB ASN 199 7.441 23.308 74.929 1.000 36.38 ANISOU 1367 CB ASN 199 4533 5029 4262 859 584 - 522 1368 CG ATOM ASN 199 7.198 22.180 73.952 1.000 31.28 ANISOU 1368 CG ASN 199 4030 4863 882 2993 202 178 ATOM 1369 OD1 ASN 199 7.743 22.151 - 72.853 1.000 37.62 ANISOU 1369 OD1 ASN 199 4693 6272 3330 122 728 - 56 MOTA 1370 ND2 ASN 199 6.393 21.190 74.314 1.000 36.42 ANISOU 1370 ND2 ASN 199 3508 1132 - 958 6251 4078 -13 MOTA 1371 N GLY 200 9.616 24.569 72.449 1.000 30.93 ANISOU 1371 N GLY 200 4342 4232 3179 436 144 -692 1372 CA GLY 200 10.920 24.304 71.866 1.000 35.26 ANISOU 1372 CA GLY 200 4430 4905 4060 -317 480 -2400 1373 C GLY 200 11.184 22.886 71.429 1.000 36.83

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ANISOU 1397 CB
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                                                     -417 1 9
                     222 14.333
MOTA
       1530 C
                VAL
                                24.965
                                       54.077 1.000 15.69
ANISOU 1530 C
                    222 1616
                VAL
                                1876
                                        2471
                                               -269 -349 -324
                    222 15.512
MOTA
       1531 0
                VAL
                                24.934 53.716 1.000 17.84
ANISOU 1531 O
               VAL
                    222 1658
                                1730
                                        3390
                                               -108 -194 4 8
       1532 CB
MOTA
               VAL
                    222 12.822 26.433 52.747 1.000 19.60
ANISOU 1532 CB
               VAL
                    222 2267
                                2202
                                        2979
                                               91 -666 -304
MOTA
       1533 CG1 VAL
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ANISOU 1533 CG1 VAL
                    222 2252
                                3113
                                        2977
                                               250
                                                     -645 -182
ATOM
       1534 CG2 VAL
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ANISOU 1534 CG2 VAL
                    222 2923
                                        3057
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                                                     -898 4 4
MOTA
       1535 N
               LEU
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ANISOU 1535 N
               LEU
                    223 1792
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                                        2706
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       1536 CA
               LEU
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ANISOU 1536 CA
                    223 1679
               LEU
                                1864
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                                               -93
                                                     -297 - 333
MOTA
       1537 C
               LEU
                    223 14.114
                                21.908
                                       53.243 1.000 14.86
ANISOU 1537 C
               LEU
                    223 1337
                                1537
                                        2773
                                               -141
                                                     -322 - 458
MOTA
      1538 O
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2132 2719 70 -391 -28
               LEU
                    223 12.969
ANISOU 1538 O
               LEU
                    223 1317
                                               70 -391 -281
ATOM
      1539 CB
               LEU
                    223 13.829
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ANISOU 1539 CB
               LEU
                    223:2740
                                1945
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MOTA
       1540 CG
                    223 14.298 20.348 55.882 1.000 23.01
223 2658 1871 4205 -375 -170 9
               LEU
ANISOU 1540 CG
               LEU
                                               -375 -170 9 1
       1541 CD1 LEU
ATOM
                    223 15.797
                                20.322 56.143 1.000 23.73
ANISOU 1541 CD1 LEU
                    223 2570
                                3067
                                        3378 69 135 3 1 6
      1542 CD2 LEU
ATOM
                    223 13.492
                                19.668 56.979 1.000 35.71
ANISOU 1542 CD2 LEU
                    223 2813
                                3296
                                        7459 525
                                                     1116 2333
MOTA
       1543 N
                    224 15.115
               VAL
                                21.370 52.570 1.000 14.18
ANISOU 1543 N
               VAL
                    224 1383
                                        2560 -28
                                1446
                                                     -320 - 205
      1544 CA
MOTA
               VAL
                    224 14.956
                                20.627 51.330 1.000 14.52
ANISOU 1544 CA
               VAL
                    224 1585
                                1501
                                        2431 -23 -323 -127
ATOM
      1545 C
               VAL
                    224 15.320 19.160 51.561 1.000 13.59
ANISOU 1545 C
               VAL
                    224 1464
                                1522
                                        2178
                                               23 -290 -251
ATOM
      1546 O
               VAL
                    224 16.442 18.861 51.981 1.000 15.38
ANISOU 1546 O
               VAL
                    224 1464
                                1558
                                        2822
                                               0 -505 -374
ATOM
       1547 CB
               VAL
                    224 15.832 21.209 50.222 1.000 14.25
ANISOU 1547 CB
               VAL
                    224 1402
                                1606
                                        2407
                                               -60
                                                    -461 - 108
      1548 CG1 VAL
ATOM
                    224 15.685 20..443 48.906 1.000 16.63
ANISOU 1548 CG1 VAL
                     224 1682
                                2164
                                        2474
                                              -159 -408 - 421
      1549 CG2 VAL
MOTA
                    224 15.575
                                22.687
                                       50.040 1.000 16.40
ANISOU 1549 CG2 VAL
                    224 1807
                                1562
                                        2863
                                               6 -509 8 7
MOTA
      1550 N
                    225 14.340
               PHE
                                18.299
                                        51.299 1.000 13.49
ANISOU 1550 N
                    225 1494
               PHE
                                        2106
                                1526
                                               -66
                                                     -353 - 130
MOTA
      1551 CA
               PHE
                    225 14.647
                                16.882
                                       51.162 1.000 14.67
ANISOU 1551 CA
               PHE
                    225 1639
                                               -115
                                                    -61 -283
                                1505
                                        2431
ATOM
      1552 C
               PHE
                    225 14.756 16.533 49.675 1.000 14.27
ANISOU 1552 C
               PHE
                     225 1536
                                1533
                                        2352
                                               100
                                                     -260 - 194
ATOM
       1553 0
               PHE
                    225 13.858 16.876 48.893 1.000 16.25
ANISOU 1553 O
               PHE
                    225 1604
                                               296
                                2000
                                        2569
MOTA
       1554 CB
               PHE
                     225-13.537
                                15.999
                                       51.749 1.000 15.57
ANISOU 1554 CB
               PHE
                     225 1613
                                1563
                                        2740
                                             -25
MOTA
       1555 CG
               PHE
                     225 13.387
                                15.996 53.257 1.000 17.95
ANISOU 1555 CG
               PHE
                     225 1888
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                                        2666 -650 -302 2 0 3
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ATOM
                     225 14.409 15.809 54.157 1.000 27.39
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- 64 -ANISOU 1556 CD1 PHE 225 2740 4234 3431 -910 -1094 900 225 12.125 15.863 53.820 1.000 21.09 1557 CD2 PHE ANISOU 1557 CD2 PHE 225 2333 2765 2917 -166 399 - 527 1558 CE1 PHE 225 14.211 15.673 55.521 1.000 26.82 ANISOU 1558 CE1 PHE 225 3108 3657 3424 -1044 -1241 1128 1559 CE2 PHE 225 11.910 15.910 55.186 1.000 21.65 ANISOU 1559 CE2 PHE 225 2994 2414 2817 623 239 - 39 1560 CZ PHE 225 12.958 15.787 56.078 1.000 28.82 ANISOU 1560 CZ PHE 225 3705 3716 3531 -832 -663 3 4 0 MOTA 1561 N CYS 226 15.795 15.817 49.266 1.000 12.77 ANISOU 1561 N CYS 226 1428 1292 2131 -60 -370 - 239ATOM 1562 CA CYS 226 15.810 15.180 47.956 1.000 12.99 226 13.610 1440 2135 12 -355 -2 0 226 14.903 13.956 47.985 1.000 12.37 226 1533 1212 1955 8 -283 -31 226 14.961 13.217 48.974 1.000 15.58 ANISOU 1562 CA CYS 12 -355 - 207 ATOM 1563 C CYS ANISOU 1563 C CYS 8 -283 -311 ATOM 1564 0 CYS ANISOU 1564 O CYS 226 1885 1651 2424 -140 -611 158 226 17.228 14.855 226 1410 1627 ATOM 1565 CB CYS 47.527 1.000 13.77 ANISOU 1565 CB CYS 2193 19 -203 - 75 ATOM 1566 SG 226 18.224 16.367 47.314 1.000 16.37 CYS ANISOU 1566 SG CYS 226 1744 1740 2735 -222 -236 -12 ATOM 1567 N GLY 227 14.150 13.722 46.928 1.000 13.20 ANISOU 1567 N GLY 227 1388 1513 2113 -28 -293 - 290MOTA 1568 CA GLY 227 13.352 12.496 46.899 1.000 12.58 ANISOU 1568 CA 227 1279 1631 1872 -83 -438 -227 13.903 11.541 45.849 1.000 12.54 GLY -83 -438 - 255 1569 C GLY ANISOU 1569 C GLY 227 1518 1279 1965 15 - 288 - 79 ATOM 1570 O GLY 227 14.917 11.732 45.152 1.000 13.58 ANISOU 1570 O GLY 227 1630 1523 2008 51 -155 8 2 ATOM 1571 N ALA 228 13.212 10.400 45.712 1.000 13.02 ANISOU 1571 N 228 1490 ALA 1306 2151 59 -204 -161 44.860 1.000 12.41 ATOM 1572 CA ALA 228 13.663 9.321 ANISOU 1572 CA ALA 228 1649 1155 1912 --- 68 -119 - 63 ATOM 1573 C ALA228 13.706 9.727 43.404 1.000 12.82 ANISOU 1573 C ALA228 1566 1288 2016 97 -223 ATOM 1574 0 ALA228 14.482 9.132 42.651 1.000 13.64 ANISOU 1574 O ALA 228 1717 1462 2004 26 -6 -131 1575 CB ALA 228 12.714 8.121 45.058 1.000 14.56 ANISOU 1575 CB ALA 228 1808 1366 2356 -219 358 -243 229 12.909 10.695 42.952 1.000 13.61 ATOM 1576 N ILE ANISOU 1576 N 229 1340 ILE 1391 2441 -43 229 13.024 11.131 41.566 1.000 12.93 ATOM 1577 CA ILE ANISOU 1577 CA 229 1325 ILE 1243 2344 ---- 4.2. -306 1 7 3 229 14.342 11.864 41.358 1.000 13.17 MOTA 1578 C ILE ANISOU 1578 C ILE 229 1327 1364 2311 -47 -191 1 3 0 MOTA 1579 0 ILE 229 14.938 11.746 40.262 1.000 14.41 ANISOU 1579 O ILE 229 1587 1596 2293 -37 -167 183 ATOM 1580 CB 229 11.768 11.888 41.103 1.000 13.46 ILE ANISOU 1580 CB ILE 229 1470 1631 2015 171 -354 - 421581 CG1 ILE ATOM 229 10.599 10.920 40.973 1.000 15.72 ANISOU 1581 CG1 ILE 229 1218 1936 2817 85 31 1 1 8 1582 CG2 ILE 229 12.040 12.674 39.808 1.000 14.19 ANISOU 1582 CG2 ILE 229 1670 1425 2298 76 - 364 174 MOTA 1583 CD1 ILE 229 10.745 9.924 39.836 1.000 20.03 ANISOU 1583 CD1 ILE 229 2129 1814 3667 -208 -385 -488 1584 N ATOM ALA 230 14.877 12.575 42.353 1.000 13.38 ANISOU 1584 N ALA 230 1252 1378 2454 -97 -176 7 4 MOTA 1585 CA ALA 230 16.209 13.185 42.130 1.000 12.30 ANISOU 1585 CA 230 1156 ALA 1444 2074 66 -97 -108 1586 C ALA 230 17.223 12.033 41.976 1.000 12.89 ANISOU 1586 C ALA 230 1491 1327 2079 128 30 - 20

- 65 -1587 0 ATOM ALA 230 18.100 12.091 41.146 1.000 13.65 ANISOU 1587 O ALA230 1240 1530 2418 103 MOTA 1588 CB ALA 230 16.588 14.000 43.345 1.000 13.66 ANISOU 1588 CB ALA230 1559 1415 2215 -186 -21 -229 ATOM 1589 N THR 231 17.143 10.978 42.805 1.000 13.31 ANISOU 1589 N THR 231 1526 1318 2214 58 - 261 - 1 ATOM 1590 CA THR 231 18.022 9.815 42.659 1.000 13.32 ANISOU 1590 CA THR 231 1660 1307 2093 78 -302 3 2 ATOM 1591 C 231 17.906 9.224 231 1300 1631 THR 41.251 1.000 13.27 2111 ANISOU 1591 C THR 205 -211 3 ATOM 1592 0 231 18.932 THR 40.620 1.000 15.51 8.974 ANISOU 1592 O THR 231 1468 1759 2667 245 58 - 170 8.751 ATOM 1593 CB THR 231 17.656 43.688 1.000 13.03 ANISOU 1593 CB THR 231 1500 1302 2151 46 -166 1 2 1594 OG1 THR ATOM 231 17.530 9.313 44.995 1.000 14.70 ANISOU 1594 OG1 THR 231 1742 1614 2230 -99 32 -14 231 18.698 7.621 43.697 1.000 13.69 1595 CG2 THR ATOM ANISOU 1595 CG2 THR 231 1449 1419 2335 113 -211 1 9 7 1596 N ATOM LEU 232 16.665 9.049 40.796 1.000 13.43 ANISOU 1596 N LEU 232 1447 1384 2271 75 -404 - 27 1597 CA LEU ATOM 232 16.446 8.396 39.527 1.000 14.11 ANISOU 1597 CA LEU 232 1809 1226 2326 80 -468 4 9 ATOM 1598 C LEU 232 16.975 9.243 38.381 1.000 15.53 ANISOU 1598 C LEU 232 1968 1557 2376 209 -3 9 0 1599 0 ATOM LEU 232 17.749 8.808 37.504 1.000 17.16 ANISOU 1599 O LEU 232 2024 1949 2546 107 -116 -519 1600 CB LEU ATOM 232 14.940 8.135 39.368 1.000 14.47 ANISOU 1600 CB LEU 232 1692 1630 2175 72 - 396 - 161 ATOM 1601 CG LEU 232 14.525 38.155 1.000 15.89 7.307 ANISOU 1601 CG LEU 232 1941 1768 2329 1<u>2</u>0 -470 - 303ATOM 1602 CD1 LEU 232 15.118 5.920 38.202 1.000 23.19 ANISOU 1602 CD1 LEU 232 3565 2020 3228 743 -1110 -851 ATOM 1603 CD2 LEU 232 13.003 232 2006 7.190 38.126 1.000 19.46 ANISOU 1603 CD2 LEU 2262 3126 -470 -523 - 66 2262 3126 -470 -523 -10.514 38.299 1.000 13.73 MOTA 1604 N 233 16.539 VAL ANISOU 1604 N VAL 233 1736 2025 -7 -263 1931454 MOTA 1605 CA VAL 233 16.893 37.117 1.000 13.84 11.317 ANISOU 1605 CA VAL 233 1674 1658 1926 141 -73 107 ATOM 1606 C VAL 233 18.407 11.510 37.025 1.000 14.08 ANISOU 1606 C VAL 233 1716 1674 1958 72 -46 1 1 3 MOTA 1607 O VAL 233 18.940 11.587 35.910 1.000 16.65 ANISOU 1607 O VAL 233 1923 2325 2079 38 109 4 0 1 ATOM 1608 CB 233 16.098 VAL 12.626 37.062 1.000 14.69 ANISOU 1608 CB VAL 233 1680 1696 2206 141 -165 3 3 3 1609 CG1 VAL ATOM 233 16.529 13.650 38.113 1.000 15.70 ANISOU 1609 CG1 VAL 233 1615 1654 2698 34 156 - 28 1610 CG2 VAL ATOM 233 16.117 13.206 35.647 1.000 16.43 ANISOU 1610 CG2 VAL 233 1740 2041 2459 251 117 596 MOTA 1611 N 234 19.100 THR 11.594 38.175 1.000 14.23 ANISOU 1611 N 234 1599 THR 1724 2083 146 -110 2 3 5 1612 CA THR MOTA 234 20.524 11.908 38.148 1.000 16.14 ANISOU 1612 CA THR 234 1664 1868 63 -171 - 49 2602 1613 C MOTA THR 234 21.346 10.621 38.006 1.000 17.09 ANISOU 1613 C THR 234 1717 1865 2912 211 - 51 146 ATOM 1614 0 THR 234 22.558 10.644 38.139 1.000 17.25 ANISOU 1614 O THR 234 1776 1951 2828 108 200 229 ATOM 1615 CB THR 234 21.030 39.373 1.000 15.29 12.681 ANISOU 1615 CB THR 234 1667 1502 2642 -46 1616 OG1 THR ATOM 234 20.849 11.819 40.522 1.000 15.45 ANISOU 1616 OG1 THR 234 1659 1708 2502 -80 1617 CG2 THR ATOM 234 20.291 13.978 39.597 1.000 16.61

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ANISOU 1617 CG2 THR 234 1564
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                                         3077
                                                3 - 34 - 42
 ATOM
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                 GLY
                      235 20.712 9.441
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 ANISOU 1618 N
                 GLY
                      235 1905
                                 1914
                                         2564
                                                193
 ATOM
        1619 CA
                GLY
                      235 21.484 8.209
                                         37.792 1.000 17.10
 ANISOU 1619 CA GLY
                      235 2049
                                 1861
                                         2586
                                                133
                                                      223 - 488
        1620 C
                GLY
                      235 22.225
                                7.931
                                         39.083 1.000 18.06
 ANISOU 1620 C
                GLY
                     235 2046
                                 2049
                                         2768
                                                419
                                                    499 3 0 3
 MOTA
        1621 0
                GLY
                     235 23.285
                                 7.289
                                         39.010 1.000 21.26
 ANISOU 1621 O
                GLY
                     235 2167
                                 2606
                                         3303
                                                679
                                                      343 - 74
 ATOM
       1622 N
                GLY
                     236 21.602
                                8.149
                                         40.237 1.000 16.17
 ANISOU 1622 N
                GLY
                     236 1663
                                 1901
                                         2582
                                                36 291 3 0 5
        1623 CA GLY
 ATOM
                     236 22.080
                                7.673
                                         41.520 1.000 17.27
 ANISOU 1623 CA GLY
                     236 2135
                                 1671
                                         2754
                                                225
                                                      28 2 2 9
 ATOM
        1624 C
                GLY
                     236 23.033 8.639
                                         42.194 1.000 16.88
 ANISOU 1624 C
                GLY
                     236 1880
                                 1890
                                         2644
                                                204
                                                     100 222
 ATOM
        1625 0
                GLY
                     236 23.692
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 ANISOU 1625 O
                GLY
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MOTA
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237 1647 1851 2957 213 -213 2

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2004 2752 72 177 9 8
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ANISOU 1626 N
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ATOM
ANISOU 1627 CA GLN
ATOM
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                GLN
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ANISOU 1628 C
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ATOM
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_{\rm L}ATOM
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                GLN
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ANISOU 1631 CG
                    237 1850
                GLN
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MOTA
       1632 CD
                GLN
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ANISOU 1632 CD
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       1633 OE1 GLN
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ATOM
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ANISOU 1634 NE2 GLN
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                                                     374 202
ATOM
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ANISOU 1635 N
                VAL
                    238 1563
                                 1804
                                        2237
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ATOM
       1636 CA
                    238 21.533 12.075 44.862 1.000 14.41
               VAL
ANISOU 1636 CA
               VAL
                    238 1535
                                 1553
                                        2388
                                               0 -44 3 2
MOTA
       1637 C
                VAL
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ANISOU 1637 C
                    238 1414
                VAL
                                 1392
                                        2346 82 55 - 149
ATOM
       1638 0
                    238 20.136 10.174 45.302 1.000 15.87
                VAL
                    238 1655
ANISOU 1638 O
                VAL
                                1639
                                        2737
                                               -218 -285 - 22
       1639 СВ
ATOM
                VAL
                    238 20.467 13.061 44.309 1.000 14.73
ANISOU 1639 CE VAL
                     238 1817
                                1626
                                        2152
                                               35 - 437 - 95
ATOM
       1640 CG1 VAL
                    238 19.805 13.764 45.489 1.000 15.70
ANISOU 1640 CG1 VAL
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                                1490
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ATOM
                    238 21.064 13.994 43.280 1.000 16.82
       1641 CG2 VAL
ANISOU 1641 CG2 VAL
                    238 1862
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                                        2812
       1642 N
ATOM
                    239 21.119 11.153 47.071 1.000 14.47
                LYS
ANISOU 1642 N
                LYS
                    239 1704
                                 1474
                                        2318
                                               14 -40 1 2
ATOM
       1643 CA
               LYS
                    239 20.470 10.360 48.104 1.000 14.43
ANISOU 1643 CA
               LYS
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ATOM
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ANISOU 1644 C
                LYS
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                                        2642
                                                     -53 232
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ATOM
       1645 0
                LYS
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                LYS
ANISOU 1646 CB
                LYS
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MOTA
                LYS
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ANISOU 1647 CG
                LYS
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- 67 -MOTA 1648 CD LYS 239 21.738 9.511 51.683 1.000 19.76 ANISOU 1648 CD LYS 239 2954 1820 2732 -123 -1234 363 1649 CE LYS 239 21.107 8.835 MOTA 52.896 1.000 22.58 ANISOU 1649 CE LYS 239 3331 2164 3086 -652 **-**1502 863 ATOM 1650 NZ LYS 239 21.904 8.883 54.145 1.000 23.13 ANISOU 1650 NZ LYS 239 2817 3360 2612 -471 -943 2 8 7 ATOM 1651 N ALA 240 18.140 9.892 48.659 1.000 14.35 ANISOU 1651 N 240 1429 1607 2418 -156 -334 - 61 240 16.791 10.192 49.145 1.000 13.98 ALA 1652 CA ALA ATOM ANISOU 1652 CA ALA 240 1468 2210 -151 -335 - 10 1635 ALA 240 16.728 9.776 ATOM 1653 C 50.605 1.000 13.44 ANISOU 1653 C ALA 240 1439 1388 2279 77 -450 2 2 ATOM 1654 0 ALA 240 16.514 8.592 50.913 1.000 16.32 ANISOU 1654 O ALA 240 1932 1567 2699 -215 -673 3 1 4 1655 CB ALA 240 15.712 9.565 ATOM 48.268 1.000 15.21 ANISOU 1655 CB ALA 240 1510 1962 2306 -104 -387 - 307 MOTA 1636 N PRO 241 16.907 10.701 51.546 1.000 14.23 ANISOU 1656 N PRO 241 1634 1551 2221 -87 -292 7 1 ATOM 1657 CA PRO 241 17.035 10.251 52.940 1.000 14.68 ANISOU 1657 CA PRO 241 1718 1681 2180 - 350 - 174 - 30 ATOM 1658 C PRO 241 15.693 9.961 53.579 1.000 13.89 ANISOU 1658 C PRO 241 1659 1581 2039 -107 -207 - 74 1659 0 PRO 10.527 53.261 1.000 17.06 MOTA 241 14.629 ANISOU 1659 O PRO 241 1698 1946 2838 17 -254 1660 CB PRO 241 17.689 11.462 53.619 1.000 16.63 ANISOU 1660 CB PRO 241 2162 1657 2501 -460 -48755ATOM 1661 CG PRO 241 17.138 12.651 52.826 1.000 16.56 ANISOU 1661 CG PRO 241-2433 1601 2258 -367 -274 3 1 ATOM 1662 CD PRO 241 17.164 12.140 51.409 1.000 14.92 ANISOU 1662 CD PRO 241 1841 1490 2339 -215 -186 - 66ARG 242 15.740 9.049 54.544 1.000 15.74

ARG 242 1914 1853 2212 -381 -308 2 0 4

ARG 242 14.574 8.772 55.376 1.000 15.50

ARG 242 1955 1863 2073 -236 -291 1 8 0

ARG 242 14.406 9.841 56.437 1.000 16.60

ARG 242 1889 2011 2407 -120 -411 - 5 1

ARG 242 15.372 10.416 56.994 1.000 18.31 ATOM 1663 N ANISOU 1663 N ATOM 1664 CA ARG ANISOU 1664 CA ARG ATOM 1665 C ANISOU 1665 C ATOM 1666 0 ANISOU 1666 O ARG 242 2041 2186 2732 -216 -559 - 180 1667 CB ARG 242 14.728 7.419 56.085 1.000 18.38 MOTA ANISOU 1667 CB ARG 242 2920 1810 2253 -486 -391 2 6 9 MOTA 1668 CG ARG 242 14.564 6.273 55.094 1.000 18.42 ANISOU 1668 CG ARG 242 2372 1873 2755 -88 162 -155 1669 CD ARG 242 14.854 4.935 55.796 1.000 23.07 ATOM ANISOU 1669 CD ARG 242 3380 2022 3366 470 -483 - 217ATOM 1670 NE ARG 242 16.334 4.954 55.991 1.000 26.69 ANISOU 1670 NE ARG 242 3498 2727 3916 444 -829 4 7 242 16.941 3.921 242 3166 2879 242 16.157 2.913 MOTA 1671 CZ ARG 56.584 1.000 27.19 ANISOU 1671 CZ ARG 4284 -297 -1143 802 1672 NH1 ARG 56.989 1.000 33.14 ANISOU 1672 NH1 ARG 242 3810 3235 5546 -316 528 726 MOTA 1673 NH2 ARG 242 18.241 3.889 56.779 1.000 31.13 ANISOU 1673 NH2 ARG 242 3043 2925 5859 227 -769 4 8 4 ATOM 1674 N HIS 243 13.188 10.057 56.872 1.000 17.55 ANISOU 1674 N HIS 243 1979 2233 2457 -165 -173 - 74 MOTA 1675 CA HIS 243 12.913 11.050 57.914 1.000 17.84 ANISOU 1675 CA HIS 243 2186 2139 2452 -260 -123 - 75 ATOM 1676 C HIS 243 11.644 10.627 58.643 1.000 17.52 ANISOU 1676 C HIS 243 2102 2084 2470 -248 -164 - 325 ATOM 1677 0 HIS 243 10.870 9.803 58.132 1.000 20.23

2593

2868

243 12.865 12.456 57.324 1.000 19.74

-551 -323 - 392

243 2226

ANISOU 1677 O

ATOM

HIS

1678 CB HIS

- 68 -ANISOU 1678 CB HIS 243 2770 2248 2482 -188 -106 8 3 HIS ATOM 1679 CG 243 11.922 12.630 56.187 1.000 22.60 ANISOU 1679 CG HIS 243 3449 2513 2624 164 1680 ND1 HIS ATOM 243 12.209 12.299 54.879 1.000 25.87 ANISOU 1680 ND1 HIS 243 4780 2575 2473 -609 -403 5 3 1681 CD2 HIS 243 10.633 13.034 56.172 1.000 29.11 ANISOU 1681 CD2 HIS 243 3220 4490 3348 121 -421 163 0 12.573 54.109 1.000 32.92 ATOM 1682 CE1 HIS 243 11.182 ANISOU 1682 CE1 HIS 243 5835 3672 3001 -1102 -1367 689 243 10.214 13.012 54.875 1.000 36.95 ATOM 1683 NE2 HIS ANISOU 1683 NE2 HIS 243 5719 4201 4119 1019 -2016 987 1684 N ATOM HIS 244 11.437 11.194 59.831 1.000 18.87 ANISOU 1684 N HIS 244 2523 24-7-7 2171 -88. -141 - 117MOTA 1685 CA HIS 244 10.302 10.801 60.649 1.000 20.83 ANISOU 1685 CA HIS 244 2802 2485 2628 171 251 272 ATOM 1687 C HIS 244 9.927 11.968 61.551 1.000 20.33 ANISOU 1686 C HIS 244 1803 2969 2953 -31 -78 - 273ATOM 1687 0 HIS 244 10.482 244 2057 13.073 61.510 1.000 21.71 ANISOU 1687 O HIS 3418 2774 -535 145 -853 1688 CB HIS 244 10.714 61.468 1.000 24.38 9.557 ANISOU 1688 CB HIS 244 4066 2644 2553 -76 -390 4 4 1 ATOM 1689 CG HIS 9.725 62.423 1.000 28.34 3498 3113 595 -727 -244 11.859 ANISOU 1689 CG HIS 244 4158 3498 3113 696 -727 - 89ATOM 1690 ND1 HIS 244 13.132 9.205 62.268 1.000 32.35 ANISOU 1690 ND1 HIS 3808 244 4012 4471 548 -485 - 8501691 CD2 HIS ATOM 244 11.928 10.391 63.609 1.000 25.21 ANISOU 1691 CD2 HIS 244 2937 4137 2505 -- 373 45 21 9 ATOM 1692 CE1 HIS 244 13.887 9.531 63.312 1.000 31.71 244 4157 4277 3613 1224 -749 -ANISOU 1692 CE1 HIS 1224 -749 - 518 MOTA 1693 NE2 HIS 244 13.1. 244 3165 244 13.146 10.263 64.150 1.000 24.52 244 3165 3517 2633 794 -82 49 2 ANISOU 1693 NE2 HIS MOTA 1694 N VAL 11.687 62.349 1.000 23.87 ANISOU 1694 N 245 2627 VAL 3119 3322 -251 531 -310 12.691 63.349 1.000 24.85 1695 CA VAL ATOM 245 8.473 ANISOU 1695 CA VAL 245 2785 3770 2883 481 149 - 293 12.079 64.735 1.000 26.03 1696 C ATOM VAL 245 8.624 ANISOU 1696 C VAL 245 3220 3112 -289 179 8 9 3558 1697 0 ATOM VAL 245 8.023 11.025 64.969 1.000 27.98 VAL 245 3120 ANISOU 1697 O 3085 4428 42 295 - 59 1698 CB VAL 245 7.020 13.114 63.099 1.000 26.02 1698 CB VAL 245 2621 3489 3777 94 -103 -56 ATOM ANISOU 1698 CB 94 -103 -569 ATOM 1699 CG1 VAL 245 6.586 245 2717 14.114 64.161 1.000 28.06 ANISOU 1699 CG1 VAL 3330 4614 159 746 -485 1700 CG2 VAL 245 6.927 13.705 61.680 1.000 30.51 ANISOU 1700 CG2 VAL 245 3564 3809 4220 1264 -305 - 33 ATOM 1701 N ALA246 9.399 12.696 65.603 1.000 28.08 ANISOU 1701 N ALA246 4338 3787 2543 -850 250 254 1702 CA ALA MOTA 246 9.567 12.316 67.003 1.000 27.45 ANISOU 1702 CA ALA 246 4363 3360 2707 275 373 292 MOTA 1703 C ALA 246 8.356 12.740 67.833 1.000 32.68 ANISOU 1703 C ALA 246 4915 4473 3031 98 880 1 9 7 MOTA 1704 0 ALA 246 7.774 13.791 67.563 1.000 29.54 ANISOU 1704 O ALA 246 3522 4283 3417 -224 875 -329 ATOM 1705 CB ALA ANISOU 1705 CB ALA 246 10.819 13.010 67.542 1.000 30.33 246 4564 3949 3011 615 -221 - 422ATOM 1706 N ALA 247 8.048 11.958 68.849 1.000 34.09 ANISOU 1706 N ALA 247 4483 5156 3311 -1190 466 3 9 3 1707 CA ALA 247 7.036 12.190 69.859 1.000 34.23 ANISOU 1707 CA ALA 247 4188 5627 3189 -1215 315 .5 1 5 247 4188 247 7.609 MOTA 1708 C ALA12.910 71.081 1.000 33.31 ANISOU 1708 C 247 5419 4684 2555 ALA249 -506 1147

- 69 -ATOM 1709 0 ALA 247 8.733 12.708 71.523 1.000 38.23 ANISOU 1709 O ALA 247 5787 4478 4259 -378 -1519 1230 1710 CB ALA 247 6.383 10.881 70.314 1.000 47.11 ANISOU 1710 CB ALA6726 247 8374 2801 -2800 1464 686 ATOM 1711 N PRO 248 6.817 13.851 71.577 1.000 42.28 ANISOU 1711 N PRO 248 5771 5458 4836 -300 933 - 97 MOTA 1712 CA PRO 248 7.256 14.581 72.773 1.000 44.85 ANISOU 1712 CA PRO 248 7568 5478 3996 -645 1413 2 1 4 1713 C MOTA 248 7.161 248 7978 PRO 13.618 73.948 1.000 49.25 ANISOU 1713 C PRO 5660 5075 -1446 552 985 ATOM 1714 0 PRO 248 6.251 12.794 74.014 1.000 45.48 ANISOU 1714 O 248 7651 PRO 5391 4237 -1127 2573 -796 ATOM 1715 CB 248 6.196 PRO 15.674 72.897 1.000 49.75 ANISOU 1715 CB PRO 248 8563 4816 5523 -513 1238 - 138 ATOM 1716 CG PRO 248 4.973 72.299 1.000 50.89 15.053 ANISOU 1716 CG PRO 248 7228 6545 -108 2210 -1064 71.114 1.000 44.69 5564 ATOM 1717 CD PRO 248 5.489 14.272 ANISOU 1717 CD 4579 PRO 248 6395 6006 937 953 - 577 ATOM 1718 N 249 8.109 ARG 13.683 74.883 1.000 48.76 ANISOU 1718 N ARG 249 9141 6341 3045 -1317 1069 - 477 1719 CA ATOM ARG 249 7.865 12.783 76.024 1.000 55.51 ANISOU 1719 CA ARG 249 10023 6914 4156 -1098 895 566 ATOM 1720 C ARG 249 6.844 13.466 76.916 1.000 46.09 ANISOU 1720 C ARG 249 5561 8382 3568 -2484 -7 1237 ATOM 1721 0 ARG 249 6.244 12.915 77.831 1.000 56.25 ANISOU 1721 O ARG 249 7572 6368 7433 -377 1799 3 9 9 5 ATOM 1722 CB ARG 249 9.177 76.721 1.000 55.24 12.459 ANISOU 1722 CB ARG 249-8950 7715 4326 705 2864 1270 -ATOM 1723 CG ARG 249 9.915 11.278 76.110 1.000 71.04 ANISOU 1723 CG ARG 249 12881 7330 6779 1135 3707 6 2 2 ATOM 1724 CD ARG 249 10.403 10.303 77.165 1.000 72.89 ANISOU 1724 CD 249 11721 ARG 7984 7991 2171 2723 4 0 9 ATOM 1725 NE ARG 249 11.124 9.162 76.580 1.000 70.73 ANISOU 1725 NE ARG 249 8627 9977 8271 2362 2650 - 266 ATOM 1726 CZ ARG 249 12.039 8.493 77.282 1.000 72.71 ANISOU 1726 CZ ARG 249 10269 9417 7942 2304 2153 1 3 3 1727 NH1 ARG ATOM 249 12.297 8.893 78.521 1.000 89.50 ANISOU 1727 NH1 ARG 249 22286 6161 5559 2015 1622 3874 ATOM 1728 NH2 ARG 249 12.682 7.462 76.761 1.000 67.68 ANISOU 1728 NH2 ARG 249 5358 10062 10295 1004 3886 2 2 1 1729 N MOTA 254 1.981 75.430 1.000 85.24 ALA18.918 ANISOU 1729 N ALA254 15501 7922 8964 -4581 -1437 2347 ATOM 1730 CA ALA 254 2.287 20.081 76.257 1.000 76.08 ANISOU 1730 CA ALA 254 12510 8110 8286 -3993 1617 1592 ATOM 1731 C 254 2.943 ALA 21.216 75.489 1.000 60.91 ANISCU 1731 C ALA 254 8383 5719 9040 -506 2886 1312 1732 0 MOTA ALA 254 4.174 21.309 75.487 1.000 72.37 ANISOU 1732 O ALA 254 8056 8109 11332 1602 4553 3381 ATOM 1733 CB ALA 254 3.264 19.667 77.351 1.000 60.48 ANISOU 1733 CB ALA254 12589 7262 3131 -866 4570 -1112 MOTA 1734 N GLY 255 2.200 22.108 74.846 1.000 54.40 ANISOU 1734 N GLY 255 8029 5451 7190 594 2922 - 940ATOM 1735 CA  $\operatorname{\mathsf{GLY}}$ 255 2.880 23.171 74.098 1.000 40.05 ANISOU 1735 CA 255 5181  $\mathsf{GLY}$ 4570 5465 1424 836 -921 ATOM 1736 C 255 3.640 GLY 22.565 72.921 1.000 38.82 ANISOU 1736 C GLY 255 4227 4772 5749 557 702 -1561 MOTA 1737 0 GLY 255 4.580 23.163 72.398 1.000 39.96 ANISOU 1737 O GLY 255 2978 5715 6491 -136 -2226 -128 MOTA 1738 N SER 256 3.164 21.387 72.509 1.000 37.29 ANISOU 1738 N SER 256 5047 4594 4527 389 11 -853 MOTA 1739 CA SER 256 3.738 20.606 71.429 1.000 35.71

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ANISOU 1739 CA SER 256 4737
ATOM 1740 C SER 256 2 983
                                4533
                                        4299 560 -501 - 919
                SER
                     256 2.983
                               20.742 70.118 1.000 34.93
ANISOU 1740 C
                               4669
                SER
                     256 4584
                                        4019
                                              -98
                                                     -85 9 1
ATOM
       1741 0
                    256 3.251
                SER
                                20.000 69.162 1.000 33.92
ANISOU 1741 O
                    256 3575
                                6107
19.136
4830
                SER
                                         3207 503
                                                     304 377
ATOM
       1742 CB
                    256 3.845
               SER
                                        71.853 1.000 30.17
ANISOU 1742 CB SER
                    256 3125
                                        3509 624
                                                     212 - 492
ATOM
       1743 OG
                               18.752
               SER
                    256 2.688
                                        72.601 1.000 61.15
ANISOU 1743 OG
               SER
                    256 2987
                                8497
                                        11750 451 1943 2630
ATOM
       1744 N
                               21.700 70.030 1.000 35.54
                SER
                    257 2.065
ANISOU 1744 N
                SER
                    257 4037
                                5989
                                        3479
                                               347
                                                     242 - 86
                    257 1.379 21.993 68.767 1.000 30.95
257 2824 5827 3109 170 672 -
257 2.378 22.538 67.760 1.000 30.63
               SER
SER
MOTA
       1745 CA
ANISOU 1745 CA
                                                    672 - 509
       1746 C
ATOM
                SER
ANISOU 1746 C
                     257 3181
257 3.359
                SER
                                5524
                                        2934 -476 765 -1297
ATOM
       1747 0
                SER
                               23.159 68.199 1.000 34.70
ANISOU 1747 O
                SER
                    257 3500
                                6070
                                        3616
                                               -829 603 -1516
       1748 CB
                    257 0.331
               SER
                                23.088 69.036 1.000 38.70
ANISOU 1748 CB
                    257 3085
               SER
                                6518
                                        5103 796
                                                     1381 4 3 5
ATOM 1749 OG
                    257 0.801
               SER
                                24.361 68.601 1.000 65.12
ANISOU 1749 OG SER
                    257 8002
                                5175
                                        11565 -999 -3375 383
       1750 N `
                                22.384 66.471 1.000 30.51
ATOM
                ARG
                    258 2.119
ANISOU 1750 N
                ARG
                    258 3668
                                5068
                                        2855
                                               -332
                                                    677 - 995
ATOM
       1751 CA
               ARG
                    258 2.997
                                22.819 65.396 1.000 28.15
ANISOU 1751 CA
               ARG
                    258 3100
                                4620
                                        2976 -106
                                                     358
ATOM
       1752 C
                ARG
                     258 2.198
                                22.913 64.096 1.000 25.64
ANISOU 1752 C
                     258 3488 3381 2872 -676 273 -
258 1.132 22.294 63.981 1.000 24.93
258 3162 3240 3070 -441 478 -
                ARG
                                                     273 - 904
       1753 0
ATOM
                ARG
ANISOU 1753 O
                ARG
                                        3070 -441 478 -560
ATOM
       1754 CB
                     258 4.175
              ARG
                              1.873
4041
20 = 1
                               21.873 65.154 1.000 27.21
ANISOU 1754 CB
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                    258 3158
                                        3141 -446 313 -1352
                                4041 3141 -446 313 -
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               ARG
ANISOU 1755 CG
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                    258 5.039 19.537 64.769 1.000 36.65
MOTA
       1756 CD
                ARG
ANISOU 1756 CD
               ARG
                    258 5937
                                3466
                                        4523 106 477 306
ATOM
       1757 NE
               ARG
                    258 4.597
                              18.176 64.411 1.000 32.42
ANISOU 1757 NE
               ARG
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                                        5089 -85
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                    258 4.633 17.777 63.143 1.000 37.32
ATOM
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               ARG
ANISOU 1758 CZ
               ARG
                     258 5670
                                2958 5553 155 680 4 3
       1759 NH1 ARG
ATOM
                     258 5.075 18.622 62.217 1.000 29.98
ANISOU 1759 NH1 ARG
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                                3435
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ATOM
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                               16.566 62.824 1.000 38.66
ANISOU 1760 NH2 ARG
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                                3151 5724
                                               -190 -1632 865
ATOM
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                THR
                    259 2.806
                                23.572 63.120 1.000 23.62
ANISOU 1761 N
                    259 2625
                THR
                                3578
                                        2771 -519 315 -1037
ATOM
       1762 CA
               THR
                    259 2.337
                                23.482 61.730 1.000 21.97
ANISOU 1762 CA THR
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                                2934
                                        2800 -36
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ATOM
       1763 C
               THR
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ANISOU 1763 C
                THR
                    259 2257
                                2663
                                        2587 -38
                                                     21 - 699
ATOM
       1764 0
                    259 4.698
                THR
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ANISOU 1764 O
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                THR
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ATOM
       1765 CB
               THR
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       1766 OG1 THR
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ANISOU 1766 OG1 THR
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                                2848
                                        3648
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       1767 CG2 THR
ATOM
                     259 0.760
                                25.408 62.331 1.000 25.17
ANISOU 1767 CG2 THR
                     259 2941
                                3229
                                        3393 726
                                                     264 - 136
ATOM
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                SER
                    260 3.234
                                22.706 59.600 1.000 20.41
ANISOU 1768 N
                SER
                    260 2386
                                2762 2609 -61 74 -80
22.515 58.551 1.000 19.33
                                        2609 -61 74 -806
MOTA
       1769 CA SER 260 4.225
ANISOU 1769 CA SER
                    260 2488
                                2459
                                        2399
                                               192 8 - 344
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1770 C
ATOM
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ANISOU 1770 C
                SER
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MOTA
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                    260 2.375
                SER
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ANISOU 1771 O
                SER
                    260 1917
                                2448
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                                              -75
                                                    -269 - 573
       1772 C.B
MOTA
               SER
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ANISOU 1772 CB
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                                2458
                                        2755
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                                                    -101 - 495
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MOTA
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                                2574
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       1774 N
                SER
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                                23.329
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ANISOU 1774 N
                SER
                    261 2189
                                2215
                                        2737
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       1775 CA
ATOM
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       1776 C
ATOM
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ANISOU 1776 C
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ATOM
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                    261 1712
               SER
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                                       3456
                                              50 -483 -781
ATOM
       1778 CB
               SER
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               SER
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       1779 OG
ATOM
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MOTA
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ANISOU 1780 N
                    262 1751
               VAL
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                                              -75 -40 -436
ATOM
       1781 CA
                    262 5.247
                                20.713 52.711 1.000 15.41
               VAL
ANISOU 1781 CA
               VAL
                    262 1871
                                1938
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MOTA
       1782 C
                    262 4.914
               VAL
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ANISOU 1782 C
               VAL
                    262 1460
                                1784
                                       2095
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MOTA
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262 1488
               VAL
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ANISOU 1783 O
               VAL
                                1900
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MOTA
       1784 CB
               VAL
                    262 4.902
                                19.307 53.253 1.000 16.87
ANISOU 1784 CB
               VAL
                    262 2144
                                2005
                                       2260
                                             165
                                                    -164 2 3
       1785 CG1 VAL
ATOM
                    262 5.567
                                18.275 52.364 1.000 20.01
ANISOU 1785 CG1 VAL
                    262 2433
262 5.335
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      1786 CG2 VAL
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ANISOU 1786 CG2 VAL
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                    263 5.894
               PHE
                                21.163 50.412 1.000 13.73
ANISOU 1787 N
                    263 1497
               PHE
                                1573.
                                       2148
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MOTA
      1788 CA
                    263 5.762
              PHE
                                21.411 48.994 1.000 13.04
ANISOU 1788 CA
              PHE
                    263 1654
                                1196
                                       2105 -12
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      1789 C
ATOM
               PHE
                    263 6.479
                                20.253 48.284 1.000 13.56
ANISOU 1789 C
               PHE
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                                       2370 -175 -98 -87
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ATOM
     1790 O
               PHE
                    263 7.732
                                20.177 48.281 1.000 13.83
ANISOU 1790 O
                    263 1415
               PHE
                                1437
                                       2403 -82
                                                    -299 - 104
ATOM
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               PHE
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                    263 1658
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MOTA
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       1794 CD2 PHE
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MOTA
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ANISOU 1795 CE1 PHE
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MOTA
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MOTA
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ATOM
       1798 N
               PHE
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ANISOU 1798 N
               PHE
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ATOM:
       1799 CA
               PHE
                    264 6.267
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ANISOU 1799 CA
               PHE
                    264 1177
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MOTA
      1800 C
               PHE
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ANISOU 1800 C PHE 264 1206 1258 2004 -121 -42 8 19.097 44.683 1.000 12.55 1273 1213 -77 -120 4 6 1258 1473 1213 -77 -120 4 6 1258 1473 1213 -77 -120 4 6 1258 1473 1213 -77 -120 4 6 1258 1473 1213 -77 -120 4 6 1258 1473 1213 -77 -120 4 6 1258 1473 1213 -77 -120 4 6 1258 1473 1213 -77 -120 4 6 1258 1473 1213 -77 -120 4 6 1258 1473 1213 -77 -120 4 6 1258 1473 1213 -77 -120 4 6 1258 1473 1213 -77 -120 4 6 1258 1473 1213 -77 -120 4 6 1258 1473 1213 1213 -77 -120 4 6 1258 1473 1213 -77 -120 4 6 1258 1473 1213 -77 -120 4 6 1258 1473 1213 -77 -120 4 6 1258 1473 1213 1210 -304 -42 6 3 1258 1473 1213 1210 -304 -42 6 3 1258 1473 1213 1210 -304 -42 6 3 1258 1473 1213 1210 -304 -42 6 3 1258 1473 1210 -304 -42 6 3 1258 1473 1210 -304 -42 6 3 1258 1473 1210 -304 -42 6 3 1258 1473 1210 -304 -42 6 3 1258 1473 1210 -304 -42 6 3 1258 1473 1210 -304 -42 6 3 1258 1473 1210 -304 -42 6 3 1258 1473 1210 1258 1473 1210 -304 -42 6 3 1258 1473 1210 1258 1473 1210 1258 1473 1210 1258 1473 1210 1258 1473 1210 1258 1473 1210 1258 1473 1210 1258 1473 1210 1258 1473 1210 1258 1473 1210 1258 1473 1210 1258 1473 1210 1258 1473 1210 1258 1473 1210 1258 1473 1210 1258 1473 1210 1258 1473 1210 1258 1473 1210 1258 1473 1210 1258 1473 1210 1258 1473 1210 1258 1473 1210 1258 1473 1210 1258 1473 1210 1258 1473 1210 1258 1473 1210 1258 1473 1210 1258 1473 1210 1258 1473 1210 1258 1473 1210 1258 1473 1210 1258 1473 1210 1258 1473 1210 1258 1473 1210 1258 1473 1210 1258 1473 1210 1258 1473 1210 1258 1473 1210 1258 1473 1210 1258 1473 1210 1258 1473 1210 1258 1473 1210 1258 1473 1210 1258 1473 1210 1258 1473 1210 1258 1473 1210 1258 1473 1210 1258 1473 1210 1258 1473 1210 1258 1473 1210 1258 1473 1210 1258 1473 1210 1258 1473 1210 1258 1473 1210 1258 1473 1210 1258 1473 1210 1258 1473 1210 1258 1473 1210 1258 1473 1210 1258 1473 1210 1258 1473 1210 1258 1473 1210 1258 1473 1210 1258 1473 1210 1258 1473 1210 1258 1473 1210 1258 1473 1210 1258 1473 1210 1258 1473 1210 1258 1473 1210 1258 1473 1210 1258 1473 1210 1258 1473 1210 1258 1473 1210 1258 1473 1210 
          ANISOU 1815 CD1 LEU 265 1518 1546 1984 84 36 1 9

ATOM 1816 CD2 LEU 265 10.971 20.458 41.449 1.000 13.14

ANISOU 1816 CD2 LEU 265 1204 1593 2197 -234 41 -204

ATOM 1817 N ARG 266 6.842 17.249 41.996 1.000 12.06

ANISOU 1817 N ARG 266 1412 127 2043 -220 -190 4
                                                                                                                                                                                                                                                                                                                          2197 -234 41 -20
     2210 125 -357 - 159
                                                                                                                                                           267 5.957 14.722
267 1413 1509
                                                                1830 C
                                                                                                                                  PRO
                                                                                                                                                                                                                                                              14.722 37.222 1.000 12.61
            ANISOU 1830 C
                                                                                                                                  PRO
                                                                                                                                                                                                                                                                                                                          1868
                                                                                                                                                                                                                                                                                                                                                                              -6 44 2 7
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- 73 -MOTA 1831 0 PRO 267 4.998 14.155 37.772 1.000 13.60 ANISOU 1831 O PRO 267 1648 1355 2164 -160 118 9 3 1832 CB PRO 267 8.238 13.761 37.599 1.000 15.30 PRO ANISOU 1832 CB 267 1435 2637 1740 -28 -169 115 MOTA 1833 CG PRO 267 8.033 12.846 38.764 1.000 15.82 ANISOU 1833 CG PRO 267 1885 1804 2324 381 -270 - 197MOTA 1834 CD PRO 267 7.872 13.746 39.965 1.000 14.73 ANISOU 1834 CD PRO 267 1803 1356 2438 311 -666 - 205 ATOM 1835 N ASN 268 5.933 15.051 35.939 1.000 13.27 ANISOU 1835 N 268 1601 ASN 1665 1777 -126 -43 -127 1836 CA ASN MOTA 268 4.800 14,709 35.073 1.000 13.72 ANISOU 1836 CA ASN 268 1793 1401 2018 -214 -236 - 71 ATOM 1837 C ASN 268 4.723 13.192 34.875 1.000 13.14 ANISOU 1837 C ASN 268 1485 1350 2156 -213 104 5 4 .268 5.702 268 1698 MOTA 1838 0 ASN 12.467 34.934 1.000 13.90 ANISOU 1838 O ASN 1416 2167 -91 123 - 36 1839 CB ASN ATOM 268 4.997 15.338 33.690 1.000 15.74 ANISOU 1839 CB ASN 268 2597 -437 1 3 5 1369 2016 -66 ATOM 1840 CG 268 5.011 ASN 16.862 33.811 1.000 15.41 ANISOU 1840 CG 268 2255 ASN 1439 2162 -17 -184471841 OD1 ASN ATOM 268 4.069 17.454 34.352 1.000 17.75 ANISOU 1841 OD1 ASN 268 2573 1686 2487 42 91 - 98 1842 ND2 ASN ATOM 17.503 33.319 1.000 16.61 268 6.066 ANISOU 1842 ND2 ASN 268 2408 1355 ~50 2546 -57 142 1843 N ATOM ALA 269 3.531 12.712 34.594 1.000 13.99 ANISOU 1843 N ALA269 1677 1467 2172 -356 -65 170 ATOM 1844 CA ALA 269 3.278 11.286 34.353 1.000 13.42 ANISOU 1844 CA ALA 269 1459 1405 2234 -208 -118 1 0 7 1845 C MOTA ALA269 4.182 10.729 33.252 1.000 13.93 ANISOU 1845 C ALA 269 1289 1538 -5 1 5 3 2466 -168 MOTA 1846 0 ALA 269 4.581 9.550 33.318 1.000 14.97 ANISOU 1846 O ALA 269 1718 1476 2494 -143 112 8 6 1847 CB ATOM ALA 269 1.806 11.051 34.008 1.000 13.76 ANISOU 1847 CB 269 1300 ALA 1474 2454 -60 -61 123 1848 N ATOM ASP 270 4.482 11.541 32.251 1.000 14.38 ANISOU 1848 N ASP 270 1688 1476 2300 -151 30 - 5MOTA 1849 CA ASP 270 5.247 11.079 31.098 1.000 14.83 ANISOU 1849 CA ASP 270 1747 1693 2194 -99 -42 6 8 ATOM 1850 C 31.227 1.000 15.68 2357 -224 143 8 ASP 270 6.749 11.287 ANISOU 1850 C 270 1714 1886 ASP 143 8 ATOM 1851 0 270 7.483 ASP 11.008 30.255 1.000 17.12 ANISOU 1851 O ASP 270 1952 2354 2200 -80 139 226 ATOM 1852 CB ASP 270 4.718 11.681 29.800 1.000 17.67 ANISOU 1852 CB ASP 270 2461 1966 2288 -75 -319 1 2 6 ATOM 1853 CG ASP 270 4.968 13.168 29.649 1.000 18.22 ANISOU 1853 CG ASP 270 2284 2024 2613 -88 -80 474 1854 OD1 ASP ATOM 270 5.386 13.826 30.607 1.000 20.55 ANISOU 1854 OD1 ASP 270 3424 1541 2844 -287 4 2 5 -47 1855 OD2 ASP ATOM 270 4.646 13.698 28.552 1.000 23.06 ANISOU 1855 OD2 ASP 270 3317 2719 2727 -49 -136 8 1 2 271 7.221 ATOM 1856 N PHE 32.413 1.000 13.93 11.668 ANISOU 1856 N PHE 271 1556 1318 2417 97 31 4 1 ATOM 1857 CA PHE 271 8.671 11.723 32.644 1.000 14.41 ANISOU 1857 CA PHE 271 1624 1430 29 2 6 3 2423 110 MOTA 1858 C PHE 271 9.275 10.349 32.325 1.000 13.31 ANISOU 1858 C PHE 271 1402 -30 28 2 1 8 1430 2225 MOTA 1859 0 PHE 271 8.790 9.340 32.870 1.000 14.91 ANISOU 1859 O PHE 271 1900 1374 2392 -26 240 192 ATOM 1860 CB PHE 271 8.942 12.146 34.098 1.000 15.57 ANISOU 1860 CB PHE 271 1700 1721 2495 -66 ATOM 1861 CG PHE 271 10.386 11.791 34.516 1.000 14.56

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- 74 -
ANISOU 1861 CG PHE 271 1729
                                 1320
                                         2485
                                                -152 34 -124
MOTA
        1862 CD1 PHE
                     271 11.460 12.369
                                         33.814 1.000 17.76
ANISOU 1862 CD1 PHE
                     271 1714
                                 1581
                                         3452
                                                -235
                                                      393 - 249
       1863 CD2 PHE
ATOM
                     271 10.698
                                10.972
                                         35.570 1.000 18.04
ANISOU 1863 CD2 PHE
                     271 2182
                                 1543
                                         3130
                                                -95
                                                      -540 172
       1864 CE1 PHE
ATOM
                     271 12.786
                                12.092
                                         34.166 1.000 17.54
ANISOU 1864 CE1 PHE
                     271 1838
                                 1700
                                         3128
                                                -291 114 -50
       1865 CE2 PHE
ATOM
                     271 11.997
                                10.609
                                         35.899 1.000 18.84
ANISOU 1865 CE2 PHE
                     271 1935
                                1646
                                         3578
                                                -392 -396 4 2 5
       1866 CZ
               PHE
                     271 13.039
                                11.154
                                        35.162 1.000 17.25
ANISOU 1866 CZ
                PHE
                     271 2444
                                1697
                                         2415
                                                -486 -19 -394
ATOM
       1867 N
                THR
                     272 10.278
                                10.298
                                        31.453 1.000 13.78
ANISOU 1867 N
                THR
                     272 1514
                                        2083
                                1641
                                                30 19 1 5 4
       1868 CA
ATOM
                THR
                     272 10.811
                                9.046
                                        30.938 1.000 13.99
ANISOU 1868 CA
                THR
                     272 1551
                                1660
                                        2105
                                                -99
                                                    83 6 7
ATOM
       1869 C
                THR
                     272 12.246
                                8.841
                                        31.410 1.000 14.71
ANISOU 1869 C
                THR
                     272 1598
                                1549
                                        2441
                                                -3 108 3 5 7
ATOM
       1870 O
                THR
                     272 13.046
                                9.808
                                        31.424 1.000 16.23
ANISOU 1870 O
                THR
                     272 1646
                                1742
                                        2780
                                               -246 5 185
       1871 CB
ATOM
                THR
                     272 10.751
                               9.117
                                        29.388 1.000 16.27
ANISOU 1871 CB
               THR
                     272 1856
                                2205
                                        2119
                                               191
                                                     125 8
       1872 OG1 THR
ATOM
                    272 9.341
                                9.221
                                        29.032 1.000 17.99
ANISOU 1872 OG1 THR
                    272 1996
                                2473
                                        2368
                                               64 -190 264
ATOM
       1873 CG2 THR
                    272 11.249
                                7.856
                                        28.723 1.000 17.94
ANISOU 1873 CG2 THR
                    272 2423
                                2167
                                        2227
                                               173
                                                     177 - 94
ATOM
       1874 N
                PHE
                    273 12.567
                                7.600
                                        31.743 1.000 14.91
ANISOU 1874 N
                PHE
                    273 1644
                                1521
                                        2499
                                               92 238 218
       1875 CA PHE
MOTA
                    273 13.894
                                7.253
                                        32.254 1.000 15.16
ANISOU 1875 CA PHE
                    273 1602
                                1813
                                        2345
                                               296
                                                    277 5
ATOM
       1876 C
               PHE
                    273 14.350
                               5.899
                                        31.724 1.000 14.69
ANISOU 1876 C
               PHE
                    273 1408
                                1647
                                        2528
                                               24 479 1 7 8
       1877 O
ATOM
               PHE
                    273 13.541
                               5.086
                                        31.262 1.000 15.91
ANISOU 1877 O
               PHE
                    273 1738
                                1767
                                        2541
                                               -115 450 119
       1878 CB
ATOM
               PHE
                    273 13.899
                               7.301
                                        33.769 1.000 15.77
ANISOU 1878 CB
               PHE
                    273 1758
                                1921
                                        2314
                                               -344
                                                     286 123
ATOM
       1879 CG
                    273 12.931
               PHE
                                        34.424 1.000 14.54
                               6.336
ANISOU 1879 CG PHE
                    273 1390
                                1726
                                        2410
                                               -95
                                                     -11 195
       1880 CD1 PHE
ATOM
                    273 11.601
                               6.743
                                        34.655 1.000 16.64
ANISOU 1880 CD1 PHE
                    273 1457
                                2343
                                        2521
                                               -24
                                                     308 362
ATOM
       1881 CD2 PHE
                    273 13.295
                               5.038
                                        34.721 1.000 15.23
ANISOU 1881 CD2 PHE
                    273 1863
                                1624
                                        2300
                                               -110
                                                     91 1 3 6
ATOM
       1882 CE1 PHE
                    273 10.719
                               5.848
                                        35.259 1.000 16.10
ANISOU 1882 CE1 PHE
                    273 1593
                                2158
                                        2365
                                               -162
                                                     292 122
       1883 CE2 PHE
                    273 12.419
                               4.148
                                        35.354 1.000 16.01
ANISOU 1883 CE2 PHE
                    273 1904
                                1980
                                        2198
                                               -139 285 181
       1884 CZ PHE
MOTA
                    273 11.109 4.559
                                        35.548 1.000 15.18
ANISOU 1884 CZ
               PHE
                    273 1843
                                2001
                                        1925
                                               -141 73 - 227
MOTA
       1885 N
                    274 15.634 5.612
               SER
                                        31.926 1.000 15.31
ANISOU 1885 N
                    274 1559
               SER
                    274 1559 1940
274 16.221 4.318
                                        2317
                                               361
                                                     383 247
       1886 CA SER
                                        31.518 1.000 15.37
ANISOU 1886 CA SER
                    274 1476
                                1723
                                               32 557 1 5 6
                                        2642
                    274 15.953 3.284
ATOM
       1887 C
               SER
                                        32.588 1.000 14.67
ANISOU 1887 C
                    274 973 1877 2726
               SER
                                            -113 265 3 0 2
MOTA
       1888 0
                    274 16.310 3.476
               SER
                                        33.770 1.000 15.98
ANISOU 1888 O
               SER
                    274 1668
                                1677
                                        2728
                                               126
                                                     143 193
ATOM
       1889 CB
               SER
                    274 17.742
                               4.556
                                        31.356 1.000 17.41
ANISOU 1889 CB
                    274 1487
               SER
                                2019
                                        3112
                                               235
                                                     945 725
       1890 OG
ATOM
               SER
                    274 18.362
                               3.280
                                        31.334 1.000 18.03
ANISOU 1890 OG
               SER
                    274 1839
                                1961
                                        3052
                                               293
                                                     840 188
       1891 N
               VAL
                    275 15.395
                               2.133
                                        32.182 1.000 15.58
ANISOU 1891 N
                    275 1646
               VAL
                                1857
                                        2417
                                               -182 461 261
```

- 75 -ATOM 1892 CA VAL 275 15.158 1.033 33.137 1.000 15.65
ANISOU 1892 CA VAL 275 1681 1800 2466 -180 261 265
ATOM 1893 C VAL 275 16.454 0.445 33.659 1.000 15.33
ANISOU 1893 C VAL 275 1805 1881 2139 116 392 -45
ATOM 1894 O VAL 275 16.623 0.280 34.871 1.000 15.68
ANISOU 1894 O VAL 275 2037 1655 2267 6 297 196
ATOM 1895 CB VAL 275 14.227 -0.004 32.483 1.000 16.05 ANISOU 1895 CB VAL 275 1635 1708 2755 -76 ANISOU 1895 CB VAL 275 1635 1708 2755 -76 405 2 1 ATOM 1896 CG1 VAL 275 14.080 -1.186 33.426 1.000 17.04 ANISOU 1896 CG1 VAL 275 2045 1688 2740 -211 230 1 5 ATOM 1897 CG2 VAL 275 12.847 0.608 32.203 1.000 18.45 ANISOU 1897 CG2 VAL 275 1650 2432 2928 -57 135 2 6 9 ATOM 1898 N PRO 276 17.437 0.093 32.844 1.000 16.21 ANISOU 1898 N PRO 276 1927 1700 2532 97 589 3 6 ATOM 1899 CA PRO 276 18.707 -0.434 33.399 1.000 18.10 ANISOU 1899 CA PRO 276 1736 2115 3025 147 616 -9 3 ATOM 1900 C PRO 276 19.382 0.541 34.321 1.000 17.52 ANISOU 1900 C PRO 276 19.98 1961 2697 97 469 2 3 9 ATOM 1901 O PRO 276 19.963 0.171 35.348 1.000 19.66 ANISOU 1901 O PRO 276 276 2015 2409 3047 24 280 4 6 8 ATOM 1902 CB PRO 276 19.590 -0.796 32.214 1.000 2 0.80 1902 CB PRO 276 19.590 -0.796 32.214 1.000 20.80 ATOM ANISOU 1902 CB PRO 276 2094 2687 3121 306 771 -276 18.852 -0.390 30.999 1.000 21.57 771 - 249ATOM 1903 CG PRO ANISOU 1903 CG PRO ATOM 1904 CD PRO ANISOU 1904 CD PRO ATOM 1903 CG PRO 276 18.852 -0.390 30.999 1.000 21.57

ANISOU 1903 CG PRO 276 2051 3098 3046 340 802 -288

ATOM 1904 CD PRO 276 17.446 -0.021 31.368 1.000 18.17

ANISOU 1904 CD PRO 276 2053 2306 2546 179 832 -318

ATOM 1905 N LEU 277 19.325 1.845 34.027 1.000 17.09

ANISOU 1905 N LEU 277 1571 1898 3025 230 511 1 0 7

ATOM 1906 CA LEU 277 19.962 2.802 34.940 1.000 19.34

ANISOU 1906 CA LEU 277 2035 2141 3171 -219 218 262

ATOM 1907 C LEU 277 19.214 2.858 36.249 1.000 18.34

ANISOU 1907 C LEU 277 1963 1958 3049 -33 -3 -3 8

ATOM 1908 O LEU 277 19.815 2.957 37.319 1.000 19.29

ANISOU 1908 O LEU 277 2466 1710 3154 -271 -188 - 2

ATOM 1909 CB LEU 277 20.094 4.178 34.291 1.000 21.41 802 - 288 832 - 318 1909 CB LEU 277 20.094 4.178 34.291 1.000 21.41 MOTA ANISOU 1909 CB LEU 277 2739 2011. 3383 14 12 2 8 7 ATOM LEU LEU 277 20.910 5.192 35.111 1.000 26.34 1910 CG 
 277
 3662
 2367
 3978
 -980
 -547
 9

 277
 22.396
 4.839
 35.069
 1.000
 38.04

 277
 3764
 3171
 7518
 -487
 -2057

 277
 20.708
 6.607
 34.631
 1.000
 31.98

 277
 4023
 2018
 6109
 -366
 508
 7
 ANISOU 1910 CG -980 -547 9 4 4 ATOM 1911 CD1 LEU ANISOU 1911 CD1 LEU 7518 -487 -2057 853 1912 CD2 LEU ANISOU 1912 CD2 LEU 6109 -366 508 732 1913 N ALA 278 17.875 2.711 36.202 1.000 17.30 1913 N ALA 278 2015 1766 2793 74 218 1 1 5 ANISOU 1913 N 1914 CA ALA 278 17.124 2.712 37.464 1.000 16.75 ANISOU 1914 CA ALA 278 2200 1566 2600 216 146 -1915 C ALA 278 17.575 1.523 38.313 1.000 16.31 ATOM ANISOU 1915 C ALA 278 1849 1553 2794 -337 -196 1 0 7 1916 O ALA 278 17.718 1.635 39.523 1.000 17.26 ATOM ANISOU 1916 O ALA 278 1963 1839 2754 -62 -53 2 ATOM 1917 CB ALA 278 15.642 2.622 37.177 1.000 17.55 ANISOU 1917 CB ALA 278 2109 1880 2679 295 195 --53 205 2679 295 195 - 11 ATOM 279 17.724 0.362 37.696 1.000 17.07 1918 N ARG 279 17.724 0.362 37.696 1.000 17.07 279 2322 1399 2766 -178 26 3 0 8 279 18.099 -0.829 38.473 1.000 16.93 279 2377 1734 2323 15 -241 2 0 3 279 19.477 -0.587 39.098 1.000 19.87 279 2491 2292 2766 -487 -384 5 4 3 279 19.687 -0.974 40.234 1.000 3 3 . 0 4 ANISOU 1918 N ARG 1919 CA ARG ANISOU 1919 CA ARG 1920 C ARG ANISOU 1920 C ARG MOTA 1921 0 ARG ANISOU 1921 O 1921 O ARG 279 3615 4823 4115 -1726 -1700 2603 1922 CB ARG 279 18.164 -2.042 37.517 1.000 20.04

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ANISOU 1922 CB
                ARG
                     279 2042
                                 1609
                                          3964
                                                108
                                                      -221 - 305
       1923 CG
                      279 16.742
                ARG
                                 -2.491
                                          37.179 1.000 20.73
ANISOU 1923 CG
                      279 2152
                ARG
                                  2728
                                          2997
                                                -98
                                                     -401 - 351
        1924 CD
                ARG
                      279 16.601
                                 -3.422
                                          35.990 1.000 24.81
ANISOU 1924 CD
                ARG
                      279 3213
                                  2982
                                          3231
                                                -1 -507
ATOM
        1925 NE
                ARG
                      279 17.575
                                 -4.484
                                         36.195 1.000 27.50
ANISOU 1925 NE
                ARG
                      279 4331
                                  2656
                                          3463
                                                355
                                                      -146 - 181
       1926 CZ
MOTA
                ARG
                      279 17.301
                                 -5.725
                                         36.620 1.000 41.33
ANISOU 1926 CZ
                      279 7720
                ARG
                                 2465
                                         5519
                                                -186 -454 - 142
MOTA
       1927 NH1 ARG
                      279 16.024
                                 -6.012
                                         36.866 1.000 40.58
ANISOU 1927 NH1 ARG
                      279 8821
                                 3012
                                         3585 -1564 507 452
       1928 NH2 ARG
                      279 18.200
                                 -6.683 36.807 1.000 53.27
ANISOU 1928 NH2 ARG
                      279 9516
                                 2227
                                         8496
                                                -127 -4607 -463
MOTA
       1929 N
                GLU
                     280 20.390 0.119
                                         38.424 1.000 19.68
ANISOU 1929 N
                GLU
                     280 2172
                                 2276
                                         3028
                                                84 324 1 3 6
ATOM
       1930 CA
                     280 21.748 0.334
                GLU
                                         38.948 1.000 20.28
ANISOU 1930 CA GLU
                     280 2046
                                 2274
                                         3385
                                                25 581 1 1 5
       1931 C
MOTA
                GLU
                     280 21.705 1.257
                                         40.182 1.000 20.67
ANISOU 1931 C
                GLU
                     280 2334
                                 1968
                                         3552
                                                -281
                                                      285 2 0
ATOM
       1932 0
                GLU
                     280 22.723 1.079
                                         40.908 1.000 26.81
ANISOU 1932 O
                GLU
                     280 2659
                                 3419
                                         4107 -37
                                                      -183 - 87
       1933 CB
ATOM
                \operatorname{\mathsf{GLU}}
                     280 22.651
                                1.029
                                         37.926 1.000 24.69
ANISOU 1933 CB
                      280 2778
                GLU
                                 2558
                                         4044
                                                -351 1022 3 0 3
       1934 CG
                GLU
                     280 22.997
                                0.342
                                         36.634 1.000 27.13
ANISOU 1934 CG
                GLU
                     280 2605
                                 4888
                                         2816
                                                596
                                                     116 623
MOTA
       1935 CD
                GLU
                     280 23.815
                                 1.298
                                         35.760 1.000 43.10
ANISOU 1935 CD
                     280 4693
                GLU
                                 7780
                                         3903
                                                -1328 1206 8 3 4
ATOM 1936 OE1 GLU
ANISOU 1936 OE1 GLU
                     280 24.541
                                 2.171
                                         36.296 1.000 41.36
                     280 2666
                                 6033
                                         7015
                                                27 1099 690
ATOM
       1937 OE2 GLU
                     280 23.727
                                 1.219
                                         34.520 1.000 64.81
ANISOU 1937 OE2 GLU
                     280 10844
                                 10028
                                         3751
                                                -2356 1104 2134
ATOM
       1938 N
                CYS
                     281 20.777 2.156
                                         40.313 1.000 21.61
ANISOU 1938 N
                CYS
                     281 2372 2240
                                         3599
                                                -211
                                                      532 - 238
ATOM
       1939 CA
                CYS
                     281 20.481 3.164
                                         41.337 1.000 24.33
ANISOU 1939 CA
                CYS
                     281 2114 2911
                                         4219 -526 1121 -817
ATOM
                     281 19.858 2.568
281 2492 3261
281 19.789 3.161
       1940 C
                CYS
                                         42.585 1.000 27.11
ANISOU 1940 C
                CYS
                                         4546 -1608 1457 -1343
ATOM
       1941 0
                CYS
                                         43.685 1.000 19.19
ANISOU 1941 O
                CYS
                     281 1997 2012
281 19.632 4.438
                     281 1997
                                         3282
                                               -250 -326 1 3 5
ATOM
       1942 CB
                CYS
                                         40.795 1.000 22.02
ANISOU 1942 CB
                CYS
                     281 1214 3088
                                         4063 -286 100 -2108
39.444 1.000 53.41
       1943 SG
ATOM
                CYS
                     281 20.639 5.092
ANISOU 1943 SG
                CYS
                     281 10822 4742
                                         4730
                                                -3261 1316 4 5
ATOM
       1944 N
                GLY
                     282 19.370 1.317
                                         42.565 1.000 18.81
ANISOU 1944 N
                GLY
                     282 1230 2224
                                         3695
                                                3 -149 -206
ATOM
       1945 CA
                GLY
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ATOM	2014				11.695	3.862	27.077	1.000 25.98
ANISOU				291	3160	4072	2641	-86 703 503
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ATOM ANISOU			THR THR		8.054	5.258	31.916	1.000 13.54
ANISOU	2021		THR		1468 7.605	1617	2058	117 373 - 118
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ANISOU	2023		THR		1565 7.407	1647	1877	152 209 - 232
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MOTA	2031		PHE	294	5.403	6.253	37.143	1.000 13.27
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ATOM	2033		PHE		6.306	9.488		1.000 13.10
ANISOU			PHE	294	1786	1216	1974	-125 -63 -244
ATOM	2034				7.207	9.411		1.000 17.41
ANISOU					2132	2533	1952	-1012 -287 7 6
ATOM ANISOU	2035	CDZ	PHE		4.964	9.739		1.000 18.41
ATOM	2036				2156	2263	2575	565 332 5 7
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ATOM	2040		GLN		3.320	6.484		1.000 12 . 76
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ATOM	2042		GLN		2.922	4.238		1.000 13.61
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ANISOU			GLN		1227	1594	2616	81 -133 192
ATOM	2044	CG	GLN		1.062	6.256		1.000 14.03

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ATOM	2045		GLN		0.157	5.687		1.000 13.56
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ATOM	2047				-0.982	6.026	32.943	1.000 15.04
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ANISOU			ASP		1628	3.016	1755	53 -51 - 151
ATOM	2050		ASP		5.167	2.569	35.792	1.000 11.57
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ATOM	2054				4.110	2.725		1.000 15.83
ANISOU	2054				1680	1935	2402	-68 -126 - 189
ATOM ANISOU	2055	002	ASP		6.212	3.098		1.000 15.27
ATOM	2056		TRP		1757	1937	2106	-229 137 177
ANISOU			TRP		6.038 1325	3.352		1.000 12.26
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ATOM	2058		TRP		5.746	3.007		-104 -49 151 1.000 13.13
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ANISOU	2062	CD1	TRP		1615	1689	2618	275 -544 - 77
ATOM	2063				9.144	4.353	40.189	1.000 14.69
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ANISOU	2065	CE2	TRP		1241	2009	2880	182 -676 - 196
ATOM	2066	CE3	TRP		9.094	5.756	40.284	1.000 22.13
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ATOM					10.318	4.180	42.316	1.000 18.45
ANISOU					2204	2387	2418	44 - 326 - 331
ATOM	2068	CZ3	TRP		9.670	6.353		1.000 21.55
ANISOU					2916	2104	3167	-55 -752 -458
ATOM	2069	CHZ	TRP	297	10.258	5.546		1.000 23.53
ANISOU ATOM	2069				3298	2356	3285	-320 -1146 -344
ANISOU			ILE		5.106	4.167		1.000 13.58
ATOM	2070		ILE	278	1324	1726	2108	241 -167 1 2 7
ANISOU			ILE		4.299 1413	4.440		1.000 14.68
ATOM	2072	CK	ILE		2.841	2177 4.054	1986	-13 -161 - 208
ANISOU			ILE		1455	1300		1.000 12.02
ATOM	2073	_	ILE		2.182	3.782	1813	56 -239 402
ANISOU			ILE	290	1732	3.782 1582		1.000 13.67
ATOM	2074		ILE		4.428	5.914	1881	-23 -4 1 9 <b>3</b> 1.000 19.45
ANISOU			ILE		2261	2446	2683	
	~ ~ . 1	22		~ > 0	~ & U I	2440	2003	-699 237 -835

	<i>,</i>			

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ATOM	2075				5.907	6.245	41.001	1.000 27.83
ANISOU	2075	CG1	ILE	298	2776	4275	3525	-1314 -556 -1030
ATOM	2076	CG2	ILE	298	3.679	6.319		1.000 25.05
ANISOU					3770	3344	2405	-57 255 -983
ATOM	2077				6.368	5.628		1.000 43.32
ANISOU				298	4561	7224	4674	-652 -1890 -117
ATOM	2078	N	GLY	299	2.317	3.980	38.893	1.000 12.16
ANISOU			GLY		1432	1308	1879	78 -304 106
ATOM	2079		GLY		0.918	3.741	38.670	1.000 12.98
ANISOU			GLY		1276	1279	2379	106 -188 -154
ATOM	2080	С	GLY	299	0.135	5.017	38.378	1.000 13.09
ANISOU	2080	С	GLY		1421	1403	2151	113 -231 1 1 8
ATOM	2081		GLY		0.738	6.025	2131	1 000 14 00
							30.01/	1.000 14.00
ANISOU			GLY		1713	1353	2252	122 289 - 13
$\mathtt{ATOM}$	2082		GLY	300	-1.183	4.917	38.447	1.000 13.08
ANISOU	2082	N	GLY	300	1325	1545	2099	146 -267 -145
ATOM	2083	CA	GLY	300	-2.075	5.966		1.000 13.45
ANISOU			GLY		1447	1521	2143	
								116 -415 - 143
ATOM	2084		GLY		-2.519	6.972		1.000 12.94
ANISOU			GLY		1098	1365	2456	-52 -407 -192
ATOM	2085	0	${ t GLY}$	300	-3.262	7.875	38.672	1.000 13.39
ANISOU	2085	Ο	GLY		1321	1342	2423	-19 -217 - 4 5
ATOM	2086		ASN		-1.973	6.845		
								1.000 13.35
ANISOU			ASN		1494	1429	2151	-225 -232 -104
ATOM	2087		ASN	301	-2.162	7.842	41.313	1.000 13.83
ANISOU	2087	CA	ASN	301	1590	1435	2230	-194 -38 -61
ATOM	2088	С	ASN		-0.837	8.254		1.000 12.46
ANISOU			ASN		1676	1268	1791	-35 -142 - 20
	2089							
ATOM			ASN		-0.007	7.405		1.000 13.89
ANISOU		_	ASN		1831	1355	2093	73 -144 - 13
ATOM	2090		ASN	301	-3.075	7.238	42.360	1.000 16.01
ANISOU	2090	СB	ASN	301	1632	1909	2542	77 224 3 1 5
ATOM	2091	CG	ASN	301	-3.942	8.199		1.000 18.23
ANISOU			ASN		1986	2508	2435	190 152 - 90
ATOM	2092							
					-4.973	8.690		1.000 17.44
ANISOU					1606	1626	3394	-21 144 -190
$\mathtt{ATOM}$	2093	ND2	ASN		-3.518	8.454	44.338	1.000 33.30
ANISOU	2093	ND2	ASN	301	2804	6923	2928	1012 -230 -1523
ATOM	2094		TYR		-0.595	9.564		1.000 12.96
ANISOU			TYR		1662	1278	1985	-69 -21 -135
ATOM	2095		TYR		0.674			
								1.000 13.48
ANISOU			TYR		1673	1259	2192	-130 -132 3 4
$\mathtt{ATOM}$	2096		TYR	302	0.768	9.269	44.078	1.000 12.63
ANISOU	2096	С	TYR	302	1413	1293	2092	53 44 1 9
ATOM	2097		TYR		-0.218	9.151		1.000 14.15
ANISOU			TYR		1332	1737	22.000	
								-65 48 - 27
ATOM	2098		TYR		0.764	11.472	42.916	1.000 13.30
ANISOU	2098	СВ	TYR	302	1635	1192	2226	-81 33 4 1
ATOM	2099	CG	TYR	302	1.159	12.143	41.619	
ANISOU	2099	CG	TYR		1586	1103	1880	-59 -25 -271
ATOM	2100							
					2.501	12.233		1.000 13.11
ANISOU					1633	1284	2066	-80 11 - 18
ATOM	2101				0.235	12.709	40.739	1.000 12.52
ANISOU					1576	1132	2049	-44 13 -127
MOTA	2102	CE1	TYR	302	2.933	12.822		1.000 12.29
ANISOU					1581	1043	2045	-185 -84 - 7.7
ATOM	2103				0.637	13.273		1.000 14.12
ANISOU					1462	1443	2458	-241 15 3 2 5
ATOM	2104		TYR		1.983	13.347		1.000 12.69 *
ANISOU			TYR		1483	1224	2113	-287 -91 1 0
ATOM	2105	ОН	TYR	302	2.376	13.866	38.013	1.000 13.42



- 82 -ANISOU 2105 OH TYR 302 1505 1469 2124 -93 33 1 4 6 2106 N 303 1.956 8.855 44.450 1.000 13.92 VAL 303 1406 303 2.355 VAL ANISOU 2106 N 1637 2246 153 88 9 9 ATOM 2107 CA VAL ANISOU 2107 CA VAL 8.336 45.746 1.000 14.51 -137 -391 - 74 303 1838 1320 2355 2108 C 303 3.498 MOTA 9.244 46.239 1.000 15.23 VAL ANISOU 2108 C VAL 303 1404 1507 2876 -102 -105 - 348 303 4.471 45.512 1.000 18.70 2109 0 VAL 9.386 ATOM 303 1859 303 2.856 3386 -239 326 -504 45.632 1.000 16.75 ANISOU 2109 O 1861 VAL 6.880 2110 CB VAL ATOM ANISOU 2110 CB VAL 303 2140 1319 2905 16 -759 -123 47.017 1.000 19.53 303 3.279 2111 CG1 VAL 6.401 303 2185 ANISOU 2111 CG1 VAL 1951 3284 232 -1054 148 303 1.723 303 2476 45.125 1.000 17.82 2112 CG2 VAL 5.956 MOTA ANISOU 2112 CG2 VAL 1442 2852 -213 -558 - 406 2113 N 304 3.349 9.900 47.378 1.000 14.07 ATOM ASN ANISOU 2113 N ASN 304 1409 1369 2566 -39 -407 - 86 304 4.317 304 1474 304 5.450 2114 CA ASN 10.928 47.772 1.000 14.31 ATOM 1387 2578 -102 -424 - 5 5 10.397 48.637 1.000 13.75 ANISOU 2114 CA ASN 2115 C MOTA ASN ANISOU 2115 C 304 1360 1487 2378 34 -274 -87 ASN 1487 2378 34 -274 - 8 10.962 48.584 1.000 14.60 2116 0 304 6.539 MOTA ASN 2116 O ASN 2117 CB ASN 304 1314 304 3.589 ANISOU 2116 O 1795 2438 -34 -55 -320 12.035 48.551 1.000 14.26 MOTA ANISOU 2117 CB ASN 304 1710 2494 6 -303 176 1214 2118 CG ASN 12.661 47.642 1.000 14.81 304 2.535 MOTA 1627 2449 23 -114 4 0 2 13.255 46.622 1.000 16.52 ANISOU 2118 CG ASN 304 1551 304 2.866 304 1896 304 1.290 ATOM 2119 OD1 ASN 1746 2636 80 19 5 8 9 12.595 48.102 1.000 18.43 2980 2463 127 -10 1 9.413 49.463 1.000 16.36 ANISOU 2119 OD1 ASN 2120 ND2 ASN MOTA ANISOU 2120 ND2 ASN 304 1560 2463 127 -10 199 305 5.175 ATOM 2121 N ILE 305 1546 305 6.173 1553 ILE 3117 -78 -503 2 6 6 ANISOU 2121 N ATOM 2122 CA ILE ANISOU 2122 CA ILE 8.890 50.407 1.000 14.85 2436 165 -277 - 40 305 1670 1537 50.352 1.000 15.78 2123 C 305 6.183 7.372 MOTA ILE ANISOU 2123 C 2914 95 -438 - 51 305 1527 ILE 1555 305 5.231 305 1463 305 5.949 49.886 1.000 17.54 MOTA 2124 O ILE 6.736 ANISOU 2124 O ILE 1789 3412 -131 -404 5 51.818 1.000 17.80 9.430 2125 CB ILE ATOM ANISOU 2125 CB ILE 305 2167 1962 2634 -23 265 -209 305 4.578 305 1716 305 6.171 2126 CG1 ILE 9.091 52.416 1.000 18.93 MOTA ANISOU 2126 CG1 ILE 2127 CG2 ILE ANISOU 2127 CG2 ILE 305 2685 1863 9.459 305 4.415 53.863 1.000 21.28 2128 CD1 ILE 305 2521 306 7.246 306 1738 306 7.424 ANISOU 2128 CD1 ILE 2662 19 452 - 71 2902 6.806 50.908 1.000 14.59 MOTA 2129 N ARG 1641 2165 52 -356 271 5.360 50.828 1.000 15.25 ANISOU 2129 N ARG 2130 CA ARG MOTA ANISOU 2130 CA ARG 306 1509 2622 139 -302 7 7 1663 4.903 52.024 1.000 15.02 2131 C MOTA ARG 306 8.234 1464 2656 133 -332 - 21 5.614 52.433 1.000 16.63 2101 2536 -219 -294 - 168 306 1588 306 9.141 ANISOU 2131 C ARG MOTA 2132 0 ARG 306 1682 ANISOU 2132 O ARG 4.943 49.532 1.000 16.31 2133 CB 306 8.135 ATOM ARG 1681 2697 -100 -270 -150 ANISOU 2133 CB ARG 306 1820 49.377 1:000 18.43 2134 CG ARG 306 8.226 3.414 MOTA 306 2476 306 8.401 1700 ANISOU 2134 CG ARG 2135 CD 3.068 ATOM ARG 306 2087 ANISOU 2135 CD ARG 1971 2880 -120 -145 -330

- 83 -2136 NE ARG 306 7.136 3.228 47.188 1.000 20.53 ANISOU 2136 NE 306 2442 ARG 2013 3345 -577 -668 -234 ATOM 2137 CZ ARG 306 6.980 3.178 45.873 1.000 20.27 306 2330 ANISOU 2137 CZ ARG 2057 3316 373 -522 2 0 306 8.086 2138 NH1 ARG 3.000 45.107 1.000 22.13 ANISOU 2138 NH1 ARG 306 2136 2580 3695 274 -589 - 723 306 5.759 2139 NH2 ARG 3.250 45.341 1.000 18.44 ANISOU 2139 NH2 ARG 306 2107 1838 259 3062 -285 8 4 307 7.898 ATOM 2140 N ARG 3.775 52.612 1.000 19.10 ANISOU 2140 N ARG 307 2716 1872 2671 -294 -607 3 2 7 2141 CA ARG ATOM 307 8.576 3.212 53.768 1.000 21.13 ANISOU 2141 CA ARG 307 3321 2201 2504 -48 -845 1 3 9 ATOM 2142 C ARG 307 9.536 2.138 53.277 1.000 23.30 ANISOU 2142 C 307 3417 2170 ARG 
 307
 3417
 2170
 3267
 181
 -1046

 307
 9.385
 1.601
 52.187
 1.000
 21.01

 307
 2574
 2355
 3052
 174
 -728
 1:

 307
 7.557
 2.522
 54.694
 1.000
 27.30

 307
 4545
 3184
 2645
 -13
 -247
 70

 307
 6.839
 3.488
 55.629
 1.000
 46.30

 307
 6310
 6374
 4907
 215
 1655
 -9

 307
 7.054
 3.085
 57.085
 1.000
 66.50

 307
 11107
 10355
 3806
 -2980
 2792
 -1

 307
 5
 989
 2
 203
 57
 531
 1.000
 78
 91
 3267 181 -1046 3 9 ATOM 2143 0 ARG ANISOU 2143 O ARG -728112ATOM2144 CB ARG ANISOU 2144 CB ARG -247 7 0 5 2145 CG ARG ATOM ANISOU 2145 CG ARG 1655 - 970 ATOM 2146 CD ARG ANISOU 2146 CD ARG 3806 -2980 2792 -1145 57.531 1.000 78.91 MOTA 2147 NE ARG 307 5.989 2.203 ANISOU 2147 NE ARG 307 11821 12833 5330 -4530 1969 - 5 ATOM 2148 CZ 307 5.987 1.285 ARG 58.479 1.000 73.67 ANISOU 2148 CZ ARG 307 7704 14382 5907 -4724 1249 1051 2149 NH1 ARG ATOM 307 7.063 1.038 59.214 1.000 80.32 ANISOU 2149 NH1 ARG 307 6613 17949 5955 -3290 2179 1 0 5 2150 NH2 ARG ATOM 307 4.872 0.597 58.707 1.000 73.74 ANISOU 2150 NH2 ARG 307 9116 2983 15919 -6954 438 -917 ATOM 2151 N 308 10.551 1.861 THR 54.113 1.000 25.61 ANISOU 2151 N THR 308 4234 2212 3285 536 -1421 -232 ATOM 2152 CA THR 308 11.308 0.640 53.822 1.000 30.02 ANISOU 2152 CA THR 308 3468 1939\_ 5998 225 -1629 -194 MOTA 2153 C THR 308 10.468 -0.611 54.030 1.000 25.42 ANISOU 2153 C THR 308 2915 2190 4552 453 -626 - 321ATOM 2154 0 THR 308 9.523 -0.768 54.787 1.000 30.10 ANISOU 2154 O THR 308 4042 3482 3912 -217 -125 614 MOTA 2155 CB 308 12.581 0.531 54.688 1.000 26.09 THR ANISOU 2155 CB THR 308 2701 3586 3626 242 -361 - 456ATOM 2156 OG1 THR 308 12.140 0.751 56.028 1.000 32.90 ANISOU 2156 OG1 THR 308 4146 4188 4167 504 745 - 495308 13.577 1.594 54.256 1.000 31.43 308 3193 4702 4047 -577 -132 -538 309 10.850 -1.591 53.217 1.000 24.73 ATOM 2157 CG2 THR ANISOU 2157 CG2 THR ATOM 2158 N SER ANISOU 2158 N 309 2934 

 309 2934
 2092
 4370
 94 -574 - 391

 309 10.199
 -2.897
 53.230 1.000 25.19

 SER ATOM 2159 CA SER ANISOU 2159 CA SER 309 3793 2464 3316 -485 451 -230 309 10.466 -3.691 54.512 1.000 24.06 309 2360 2888 3893 302 107 3 MOTA 2160 C SER ANISOU 2160 C SER 107 3 5 ATOM 2161 0 SER 309 11.565 -3.621 55.084 1.000 34.54 ANISOU 2161 O SER 309 3626 2131 7366 -76 -1944 - 342162 CB SER MOTA 309 10.639 -3.700 52.012 1.000 26.52 ANISOU 2162 CB SER 309 3970 2159 3948 580 - 366 167 ATOM 2163 OG SER 309 10.217 -5.039 52.148 1.000 26.34 ANISOU 2163 OG SER 309 3198 2207 4604 156 -844 - 260MOTA 2164 N LYS 310 9.494 -4.458 54.961 1.000 24.99 ANISOU 2164 N 310 3172 LYS 2459 3864 160 262 366 2165 CA LYS ATOM 310 9.651 -5.339 56.125 1.000 28.38 ANISOU 2165 CA LYS 310 4191 3167 3427 764 278 281 MOTA 2166 C LYS 310 9.941 -6.768 55.711 1.000 26.07

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ANISOU 2166 C
                 LYS
                      310 3371
                                  2687
                                          3846 168
                                                       -290 5 7 7
                      310 10.150 -7.684 56.515 1.000 33.48
ATOM
        2167 0
                 LYS
ANISOU 2167 O
                 LYS
                      310 5267
                                  3056
                                          4400
                                                 -66
                                                       -450 1073
       2168 CB
ATOM
                LYS
                      310 8.299
                                  -5.367 56.858 1.000 37.77
ANISOU 2168 CB
                LYS
                      310 5736
                                  4695
                                          3921
                                                 299
                                                       1818 1 8
       2169 CG
                LYS
                      310 8.014
                                  -4.214 57.806 1.000 40.55
ANISOU 2169 CG
                LYS
                      310 6395
                                  4716
                                          4295
                                                 1525
                                                       1524 1 0 1
ATOM
       2170 CD
                LYS
                      310 6.798
                                  -4.587
                                         58.649 1.000 44.24
ANISOU 2170 CD
                LYS
                      310 9091
                                  4224
                                          3495
                                                 1053
                                                       2816 5 8 4
ATOM
       2171 CE
                LYS
                      310 6.722
                                  -6.109
                                         58.818 1.000 59.12
ANISOU 2171 CE
                LYS
                      310 9281
                                  4577
                                          8606
                                                 766
                                                       -82 2478
ATOM
       2172 NZ
                LYS
                     310 6.088
                                  -6.563
                                         60.089 1.000 55.80
ANISOU 2172 NZ
                LYS
                     310 4884
                                  5742
                                          10577
                                                 287
                                                       -947 4796
ATOM
       2173 N
                ALA
                     311 9.896
                                  -7.030 54.410 1.000 22.45
ANISOU 2173 N
                     311 2190
                ALA
                                  2402
                                          3939
                                                 10 52 2 6 9
ATOM
       2174 CA
                     311 10.360
311 3771
                ALA
                                 -8.369 53.972 1.000 31.89
ANISOU 2174 CA
                ALA
                                  2594
                                         5753 434
                                                       -516 - 421
                     311 11.909
311 3907
311 9.619
ATOM
       2175 C
                ALA
                                 -8.459 53.833 1.000 23.30
ANISOU 2175 C
                ALA
                                  2328
                                         2616 1393 -593 1 1 2
ATOM
       2176 CB
                ALA
                                  -8.665 52.674 1.000 27.94
ANISOU 2176 CB
                     311 2407 2878 5329 -355 542 -
501 -6.477 10.237 44.256 1.000 15.66
502 -9.349 16.189 51.010 1.000 19.26
                ALA
                                                       542 -672
ATOM
       2177 OW HOH
ATOM
       2178 OW HOH
ATOM
       2179 OW
                HOH
                     503 -1.489 3.653
                                         34.560 1.000 15.78
ATOM
       2180 OW
                HOH 504 -10.499 18.731
                                         50.182 1.000 16.19
ATOM
       2181 OW
                    505 -8.612 16.958 47.640 1.000 17.30
                НОН
ATOM
       2182 OW
                НОН
                     506 -10.255 20.839 42.881 1.000 19.05
ATOM
       2183 OW
                нон
                     507 2.096
                                         32.810 1.000 29.32
                                 1.076
ATOM
       2184 OW
                HOH
                     508 -0.284 4.743
                                         41.885 1.000 13.93
ATOM
       2185 OW
                     509 -8.525 18.553 42.416 1.000 21.33
                HOH
ATOM
       2186 OW
                нон
                     510 3.165
                                 2.604
                                         43.488 1.000 24.59
ATOM
       2187 OW
                HOH
                     511 -6.282
                                 19.386 52.341 1.000 18.98
ATOM
       2188 OW
                HOH
                     512 -6.826
                                 24.638
                                         46.833 1.000 21.77
ATOM
       2189 OW
                HOH
                     513 10.510
                                 -4.344
                                         46.092 1.000 25.88
ATOM
       2190 OW
                HOH
                     514 -0.806
                                 16.964
                                         40.372 1.000 16.54
       2191 OW
ATOM
                HOH
                     515 -1.269
                                 18.855
                                         42.411 1.000 15.76
       2192 OW
MOTA
                нон
                     516 14.277
                                 -5.146
                                         40.175 1.000 15.53
ATOM
       2193 OW
                HOH
                     517 -0.123
                                 21.538
                                         40.640 1.000 17.22
ATOM
       2194 OW
                HOH
                     518 13.131
                                 -0.967
                                         51.791 1.000 31.17
ATOM
       2195 OW
                HOH
                     519 11.009
                                 2.875
                                         45.599 1.000 20.20
ATOM
       2196 OW
                HOH
                     520 5.789
                                         45.996 1.000 17.36
                                 13.543
ATOM
      .2197 OW
                НОН
                     521 2.168
                                 19.767
                                         55.925 1.000 20.41
       2198 OW
ATOM
                HOH
                     522 8.487
                                 15.960
                                         34.949 1.000 15.40
MOTA
       2199 OW
                НОН
                     523 10.794 12.697
                                         29.921 1.000 19.99
ATOM
       2200 OW
                     524 -11.722 19.112
                HOH
                                         44.516 1.000 19.82
ATOM
       2201 OW
               нон
                     525 1.672
                                 -2.081
                                         35.124 1.000 16.29
ATOM
       2202 OW
                HOH
                     526 9.651
                                 15.283
                                         32.342 1.000 20.37
       2203 OW
ATOM
                HOH
                     527 28.749
                                 31.187
                                         52.019 1.000 18.53
ATOM
       2204 OW
                НОН
                    528 15.326
                                 11.252
                                         32.041 1.000 19.60
ATOM
       2205 OW
                НОН
                    529 26.897
                                 26.984
                                         52.035 1.000 19.86
ATOM
       2206 OW
                НОН
                    530 13.528
                                 11.592
                                         50.915 1.000 16.17
MOTA
       2207 OW
                НОН
                    531 25.631
                                 32.409
                                         52.682 1.000 19.20
ATOM
       2208 OW
                     532 18.287
                HOH
                                 6.835
                                         52.185 1.000 18.49
ATOM
       2209 OW
                HOH
                     533 12.635
                                 29.035
                                         39.395 1.000 18.09
ATOM
       2210 OW
                НОН
                     534 10.797
                                 31.968
                                         45.659 1.000 20.66
MOTA
       2211 OW
                     535 10.167
                HOH
                                 24.890
                                         33.567 1.000 19.12
ATOM
       2212 OW
                нон
                     536 23.530
                                 24.122
                                         58.531 1.000 20.39
ATOM
       2213 OW
                HOH
                     537 23.358
                                 12.639
                                         35.292 1.000 22.61
MOTA
       2214 OW
               НОН
                     538 25.879
                                 28.699
                                         50.264 1.000 19.44
MOTA
       2215 OW
                НОН
                     539 11.674
                                 16.559
27.775
                                         30.502 1.000 18.57
ATOM
       2216 OW
                HOH
                     540 18.515
                                         40.042 1.000 22.23
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ATOM 2217 OW НОН 541 21.233 20.367 33.996 1.000 21.45 ATOM 2218 OW нон 542 22.826 32.643 53.094 1.000 19.38 ATOM 2219 OW HOH 543 19.670 22.387 35.310 1.000 20.05 ATOM 2220 OW HOH 544 -13.591 21.996 61.494 1.000 49.93 ATOM 2221 OW HOH 545 21.295 11.783 55.080 1.000 20.04 2222 OW MOTA нон 51.677 1.000 28.11 546 5.431 2.533 ATOM 2223 OW нон 547 17.311 25.489 32.148 1.000 24.38 ATOM 2224 OW нон 548 17.427 7.744 33.008 1.000 20.78 нон MOTA 2225 OW 549 11.656 23.874 58.194 1.000 23.39 MOTA 2226 OW HOH 550 8.037 14.987 53.326 1.000 33.52 2227 OW ATOM HOH 551 1.354 14.574 33.889 1.000 21.05 552 11.203 553 2.671 2228 OW ATOM HOH 20.116 63.686 1.000 24.59 2229 OW 21.240 19.832 ATOM HOH 34.245 1.000 34.51 ATOM 2230 OW HOH 554 6.339 30.751 1.000 26.36 ATOM 2231 OW HOH 555 26.611 24.519 55.570 1.000 21.22 556 27.669 17.156 MOTA 2232 OW нон 53.039 1.000 25.86 ATOM 2233 OW HOH 557 -14.392 19.977 44.154 1.000 25.03 MOTA 2234 OW HOH558 14.828 32.652 51.443 1.000 25.23 2235 OW MOTA нон 559 17.937 7.207 54.915 1.000 20.59 MOTA 2236 OW HOH 560 10.729 -8.875 31.499 1.000 24.65 ATOM 2237 OW HOH 561 6.455 2.298 42.613 1.000 22.74 MOTA 2238 OW НОН 562 13.784 31.245 44.166 1.000 27.75 ATOM 2239 OW HOH 563 17.292 33.470 53.556 1.000 25.28 2240 OW ATOM HOH 564 11.210 1.109 49.697 1.000 23.33 ATOM 2241 OW HOH 565 -11.339 25.246 41.370 1.000 26.08 38.242 1.000 30.07 ATOM 2242 OW 566 20.363 нон -8.375 567 3.890 ATOM 2243 OW 35.837 1.000 25.86 43.937 1.000 25.45 HOH 24.604 ATOM 2244 OW HOH 568 5.334 11.875 ATOM 2245 OW HOH 569 7.861 22.385 64.046 1.000 28.98 ATOM 2246 OW HOH 570 7.754 30.848 1.000 24.72 -1.508 ATOM 2247 OW 28.471 1.000 33.06 51.855 1.000 30.09 HOH 571 6.297 3.583 ATOM 2248 OW HOH 572 -15.790 28.800 ATOM 2249 OW нон 573 -5.388 20.310 38.883 1.000 23.64 2250 OW ATOM HOH 574 17.657 21.059 29.053 1.000 24.31 ATOM 2251 OW нон 575 8.763 20.920 66.102 1.000 24.81 MOTA 2252 OW HOH 576 10.135 27.617 58.357 1.000 25.12 2253 OW ATOM нон 577 7.795 1.060 29.730 1.000 29.00 2254 OW ATOM HOH 578 22.601 19.580 61.946 1.000 28.66 ATOM 2255 OW HOH 579 8.859 4.744 27.898 1.000 26.12 ATOM 2256 OW нон 580 4.937 48.882 1.000 26.29 35.057 1.000 23.31 3.932 ATOM 2257 OW HOH 581 17.096 5.891 MOTA 2258 OW HOH 582 -16.337 31.047 64.719 1.000 54.01 583 7.652 ATOM 2259 OW HOH 24.826 52.106 1.000 27.23 ATOM 2260 OW HOH 584 7.174 24.915 29.292 1.000 26.60 ATOM 2261 OW HOH585 23.452 55.439 1.000 26.42 10.614 2262 OW ATOM HOH58.676 1.000 27.15 586 12.640 26.413 ATOM 2263 OW нон 587 6.204 21.166 62.094 1.000 24.65 ATOM 2264 OW нон 588 2.385 0.810 37.616 1.000 19.92 MOTA 2265 OW 589 32.930 нон 28.236 45.738 1.000 38.29 ATOM 2266 OW HOH 590 -12.045 28.716 45.065 1.000 30.46 ATOM 2267 OW HOH 13.612 36.120 1.000 27.12 591 0.219 ATOM 2268 OW 43.344 1.000 26.67 HOH 592 -2.525 3.881 ATOM 2269 OW 593 7.533 HOH 13.297 48.055 1.000 19.59 MOTA 2270 OW HOH 594 -1.575 28.355 42.057 1.000 25.53 MOTA 2271 OW -1.188 HOH 595 11.209 46.425 1.000 22.12 ATOM 2272 OW 596 5..684 нон -7.000 28.451 1.000 27.97 ATOM 2273 OW HOH 597 28.868 19.406 51.825 1.000 27.72 MOTA 2274 OW 598 13.432 HOH 2.493 57.904 1.000 31.12 MOTA 2275 OW HOH 599 8.196 27.148 1.000 29.99 7.483 MOTA 2276 OW нон 600 20.809 63.369 1.000 36.86 19.088 ATOM 2277 OW нон 601 21.352 10.656 34.614 1.000 30.60

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- 86 -2278 OW HOH ATOM 602 2.891 7.196 30.899 1.000 25.41 2279 OW ATOM HOH 603 8.260 26.496 34.561 1.000 35.71 ATOM 2280 OW HOH 604 22.300 13.959 31.378 1.000 32.53 ATOM 2281 OW НОН 605 15.689 48.870 1.000 31.17 35.750 ATOM 2282 OW HOH 606 7.219 15.638 30.914 1.000 27.80 ATOM 2283 OW нон 607 -3.237 14.604 47.092 1.000 20.96 ATOM 2284 OW · HOH 608 17.543 10.581 33.561 1.000 23.51 ATOM 2285 OW HOH 609 -1.899 36.370 44.261 1.000 32.64 ATOM 2286 OW HOH 610 26.095 14.431 43.803 1.000 19.19 ATOM 2287 OW HOH 611 27.664 13.183 41.954 1.000 26.48 ATOM 2288 OW нон 612 4.302 34.604 49.981 1.000 24.70 ATOM 2289 OW HOH 613 -15.580 27.012 46.728 1.000 42.45 ATOM 2290 OW HOH 614 1.615 35.544 50.347 1.000 23.78 ATOM 2291 OW HOH 615 -10.137 34.259 49.033 1.000 23.94 ATOM 2292 OW HOH 616 26.084 6.502 57.657 1.000 39.32 2293 OW ATOM HOH 617 -15.962 20.656 46.340 1.000 25.94 ATOM 2294 OW HOH 618 6.113 29.517 40.143 1.000 29.43 ATOM 2295 OW нон 619 19.797 51.313 1.000 27.15 4.627 ATOM 2296 OW HOH 620 -1.748 11.315 48.716 1.000 21.83 ATOM 2297 OW нон 621 11.099 34.289 44.259 1.000 27.15 2298 OW ATOM 622 28.352 HOH 14.351 37.877 1.000 41.48 MOTA 2299 OW 623 -2.826 HOH 36.968 57.149 1.000 32.75 ATOM 2300 OW 624 16.983 625 16.780 HOH 9.258 29.962 1.000 32.82 ATOM 2301 OW HOH 29.213 38.384 1.000 27.96 MOTA 2302 OW нон 626 1.632 17.213 733.689 1.000 23.17 ATOM 2303 OW 627 33.536 HOH 23.640 45.028 1.000 41.91 ATOM 2304 OW НОН 628 23.821 50.174 1.000 34.22 46.751 1.000 39.07 6.059 2305 OW ATOM HOH 629 3.482 2.785 2306 OW ATOM 630 20-218 24.803 HOH 60.918 1.000 50.12 ATOM 2307 OW HOH 631 3.366 30.698 1.000 31.50 16.272 ATOM 2308 OW нон 632 18.871 11.791 31.384 1.000 30.78 2309 OW ATOM HOH 633 4.455 25.782 58.823 1.000 32.14 ATOM 2310 OW 634 24.721 НОН 40.319 1.000 40.13 5.202 ATOM 2311 OW HOH 635 19.623 35.238 43.466 1.000 50.48 ATOM 2312 OW 636 22.789 26.242 6<u>3</u>7 7.008 -4.809 HOH 60.797 1.000 26.58 MOTA 2313 OW HOH -4.809 54.039 1.000 33.89 MOTA нон 638 -15.821 18.362 639 -11.847 15.711 2314 OW 42.559 1.000 29.61 ATOM 2315 OW нон 52.841 1.000 25.21 MOTA 2316 OW нон 640 -1.948 13.411 35.401 1.000 30.41 ATOM 2317 OW нон 641 -14.293 21.937 42.145 1.000 27.58 MOTA 2318 OW HOH 642 18.216 20.839 66.863 1.000 31.23 2319 OW MOTA HOH 643 9.836 36.288 48.178 1.000 44.21 MOTA 2320 OW HOH 644 3.510 16.168 66.253 1.000 33.82 MOTA 2321 OW нон 645 7.571 41.687 1.000 37.96 33.398 MOTA 2322 OW HOH 646 0.780 21.844 36.729 1.000 31.71 ATOM 2323 OW НОН 647 21.244 -2.321 35.579 1.000 32.40 MOTA 2324 OW HOH 648 3.027 69.907 1.000 36.84 25.244 ATOM 2325 OW HOH 649 1.129 25.273 66.516 1.000 35.42 MOTA 2326 OW HOH 650 14.646 7.560 60.327 1.000 46.42 MOTA 2327 OW HOH 651 -8.287 26.381 37.998 1.000 29.17 MOTA 2328 OW HOH 652 10.153 23.548 67.703 1.000 31.50 MOTA 2329 OW 653 28.906 HOH 22.258 38.969 1.000 32.66 ATOM 2330 OW нон 654 13.568 -4.482 31.517 1.000 26.94 ATOM 2331 OW HOH 655 -12.635 17.106 55.637 1.000 26.85 50.702 1.000 29.05 ATOM 2332 OW HOH. 656 2.698 5.770 2333 OW ATOM 657 -1.384 HOH 7.487 46.512 1.000 36.52 MOTA 2334 OW 658 3.880 HOH 19.246 31.498 1.000 31.50 MOTA 2335 OW HOH 659 -1.400 31.406 64.001 1.000 56.62 MOTA 2336 OW НОН 660 11.416 23.260 65.229 1.000 32.69 MOTA 2337 OW HOH 661 15.994 14.673 25.680 1.000 36.46 ATOM

21.242 53.423 1.000 39.06

662 28.572

2338 OW

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2339 OW ATOM HOH 663 19.354 0.465 27.273 1.000 44.56 MOTA 2340 OW нон 27.026 38.838 1.000 35.41 664 24.969 ATOM 2341 OW HOH 665 24.294 7.488 55.914 1.000 32.97 ATOM 2342 OW нон 666 19.540 7.882 31.178 1.000 30.04 ATOM 2343 OW нон 32.988 57.241 1.000 39.20 667 -9.236 ATOM 2344 OW нон 668 2.098 18.351 67.496 1.000 38.83 ATOM 2345 OW HOH 669 11.390 3.245 56.270 1.000 37.56 2346 OW ATOM нон 670 -21.413 24.449 52.026 1.000 44.66 ATOM 2347 OW 671 -14.575 19.220 672 32.112 25.958 - HOH 55.240 1.000 30.91 ATOM 2348 OW HOH 43.051 1.000 33.34 2349 OW MOTA 673 -15.050 31.151 HOH 53.232 1.000 34.71 674 2.941 30.245 1.000 34.63 34.757 1.000 49.17 39.386 1.000 30.55 2350 OW ATOM HOH -1.607MOTA 2351 OW нон 675 26.951 14.544 ATOM 2352 OW HOH 676 14.707 30.669 2353 OW ATOM НОН 18.009 68.080 1.000 43.41 677 5.203 2354 OW ATOM 678 14.151 HOH 7.965 26.591 1.000 38.80 ATOM 2355 OW HOH 679 24.470 24.251 41.443 1.000 31.28 2356 OW ATOM HOH 680 17.540 2.410 28.478 1.000 34.31 ATOM 2357 OW 681 25.992 20.593 34.326 1.000 39.66 НОН ATOM 2358 OW HOH 682 13.802 35.357 44.421 1.000 34.06 2359 OW ATOM HOH 683 1.087 2.355 45.456 1.000 35.39 2360 OW ATOM 684 22.443 34.538 42.053 1.000 33.55 HOH ATOM 2361 OW HOH 4.720 685 4.419 27.356 1.000 48.02 ATOM 2362 OW HOH 686 -15.830 34.507 687 -15.217 29.490 51.877 1.000 50.63 ATOM 2363 OW HOH 48.887 1.000 33.54 ATOM 2364 OW HOH 688 36.808 21.183 46.206 1.000 44.97 ATOM 2365 OW нон 689 3.756 1.312 29.272 1.000 35.16 ATOM 2366 OW HOH 690 18.802 13.646 27.901 1.000 30.08 ATOM 2367 OW 17.521 HOH 691 6.997 29.313 1.000 47.70 ATOM 2368 OW 692 13.725 HOH 16.327 69.105 1.000 36.97 2369 OW ATOM HOH 693 22.369 60.503 1.000 44.09 22.161 MOTA 2370 OW нон 694 -5.429 31.620 42.219 1.000 33.40 MOTA 2371 OW HOH 695 19.351 23.082 30.744 1.000 34.21 2372 OW ATOM HOH 696 6.897 22.414 29.376 1.000 36.59 ATOM 2373 OW HOH 697 28.700 7.809 57.304 1.000 38.35 ATOM 2374 OW HOH 698 3.224 0.679 39.819 1.000 24.13 ATOM 2375 OW 699 -4.634 HOH 33.717 62.593 1.000 32.26 2376 OW ATOM HOH 700 32.423 17.018 43.200 1.000 43.20 68.342 1.000 39.95 2377 OW ATOM 25.228 HOH 701 12.119 MOTA 2378 OW HOH 702 9.307 28.976 1.000 31.75 1,6.477 ATOM .. 2379 OW HOH 703 -11.313 34.067 46.117 1.000 49.40 2380 OW ATOM HOH 704 7.774 31.390 65.371 1.000 39.12 ATOM 2381 OW нон 705 24.764 7.530 36.802 1.000 38.55 2382 OW ATOM HOH 706 -22.095 25.669 59.047 1.000 36.71 2383 OW MOTA НОН 707 14.509 9.840 68.854 1.000 50.38 ATOM 2384 OW нон 708 -10.129 28.722 42.036 1.000 38.92 MOTA 2385 OW нон 709 29.011 34.910 48.390 1.000 35.29 ATOM 2386 OW 710 15.822 НОН 31.612 42.021 1.000 33.61 ATOM 2387 OW HOH 711 -1.996 17.676 33.645 1.000 49.57 ATOM 2388 OW 712 10.216 HOH 17.748 26.015 1.000 41.04 ATOM 2389 OW HOH 713 23.535 29.642 37.371 1.000 43.47 MOTA 2390 OW НОН 714 20.488 -7.214 35.599 1.000 45.99 ATOM 2391 OW нон 715 11.411 10.149 25.081 1.000 41.63 ATOM 2392 OW HOH 716 19.329 -4.258 34.139 1.000 42.50 ATOM 2393 OW HOH 717 13.688 26.799 66.321 1.000 43.74 ATOM 2394 OW HOH 718 -10.751 33.064 54.747 1.000 40.47 2395 OW ATOM 719 13.800 HOH 18.258 70.756 1.000 34.54 ATOM 2396 OW HOH 720 17.151 5.815 28.003 1.000 40.80 ATOM 2397 OW нон 721 0.000 0.000 36.691 0.330 27.42 ATOM 2398 OW нон 722 0.000 0.000 41.559 0.330 37.77 ATOM 2399 OW нон 723 15.314 7.549 28.791 1.000 36.24

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MOTA 2400 OW HOH 724 -1.663 19.944 39.196 1.000 33.87 ATOM 2401 OW HOH 725 19.289 24.195 33.321 1.000 32.28 ATOM 2402 OW HOH 726 0.000 0.000 31.798 0.330 50.38 ATOM 2403 OW HOH 727 -1.223 38.165 59.229 1.000 31.24 ATOM 2404 OW HOH 728 22.035 38.254 45.742 1.000 48.21 ATOM 2405 OW HOH 729 28.388 16.248 63.044 1.000 31.59 ATOM 2406 OW HOH 730 0.000 0.000 45.995 0.330 36.14 НОН MOTA 2407 OW 731 2.984 29.007 40.091 1.000 36.08 MOTA 2408 OW HOH 732 5.297 27.318 1.000 41.53 15.835 ATOM 2409 OW HOH 733 17.347 10.778 27.373 1.000 35.27 ATOM 2410 OW HOH 734 29.417 14.607 53.127 1.000 40.12 ATOM 2411 OW HOH 735 4.222 -8.636 27.012 1.000 35.22 ATOM 2412 OW HOH 736 -9.949 17.712 62.813 1.000 34.43 ATOM 2413 OW HOH 737 13.960 -10.203 55.259 1.000 31.79 ATOM 2414 OW HOH 738 11.831 49.308 1.000 25.22 -1.522 ATOM 2415 OW HOH 739 2.896 4.247 29.596 1.000 38.64 ATOM 2416 OW HOH 740 10.959 13.759 25.528 1.000 61.86 ATOM 2417 OW HOH 741 0.864 17.227 30.557 1.000 50.71 ATOM 2418 OW HOH 742 31.755 18.949 52.065 1.000 40.48 ATOM 2419 OW HOH 743 21.678 -0.485 28.218 1.000 43.23 ATOM 2420 OW HOH 744 10.583 16.397 75.211 1.000 45.04 ATOM 2421 OW HOH 745 7.480 7.996 78.287 1.000 57.64 ATOM 2422 OW HOH 746 24.067 35.122 40.297 1.000 41.95 ATOM 2423 OW HOH 747 7.804 10.269 78.332 1.000 49.63 ATOM 2424 OW HOH 748 22.131 40.645 45.806 -1.000 49.69 ATOM 2425 OW HOH 749 14.850 -4.647 33.872 1.000 42.88 ATOM 2426 OW HOH 750 -12.930 32.504 55.211 1.000 37.15 ATOM 2427 OW HOH 751 -4.832 35.986 43.333 1.000 44.39 ATOM 2428 OW HOH 752 19.834 33.566 56.449 1.000 31.56 ATOM 2429 OW HOH 753 3.363 22.310 29.844 1.000 42.02 ATOM 2430 OW HOH 754 25.594 4.030 34.174 1.000 51.90 ATOM 2431 OW HOH 755 28.036 35.859 46.448 1.000 39.50 ATOM 2432 OW HOH 756 -12.951 16.294 61.787 1.000 40.94 MOTA 2433 OW HOH 757 -10.870 26.452 38.737 1.000 44.85 ATOM . 2434 OW HOH 758 13.216 12.896 70.729 1.000 63.42 ATOM 2435 OW HOH 759 -0.403 21.161 74.990 1.000 38.96 ATOM 2436 OW HOH 760 -7.025 32.526 64.316 1.000 39.64 ATOM 2437 OW HOH 761 -15.459 19.739 58.090 1.000 40.84 MOTA 2438 OW HOH 762 -4.964 36.577 59.068 1.000 48.64 ATOM 2439 OW HOH 763 26.807 35.717 50.036 1.000 43.54 MOTA 2440 OW HOH 764 19.542 7.083 65.538 1.000 41.41 MOTA 2441 OW HOH 765 3.709 35.837 42.709 1.000 33.78 ATOM 2442 OW нон 766 0.431 33.688 40.172 1.000 36.91 ATOM 2443 OW HOH 767 18.620 5.064 64.617 1.000 45.76 ATOM 2444 OW HOH 768 35.526 19.792 41.322 1.000 52.54 ATOM 2445 OW HOH 769 19.671 7.789 67.717 1.000 43.44 **ATOM** 2446 OW HOH 770 3.562 12.048 26.149 1.000 40.08 ATOM 2447 OW HOH 771 20.245 35.637 53.927 1.000 52.16 ATOM 2448 OW HOH 772 -20.588 25.640 61.573 1.000 58.60 2449 **ATOM** OW HOH 773 1.556 37.342 52.171 1.000 36.23 ATOM 2450 OW HOH 774 8.340 0.668 49.382 1.000107.24 ATOM 2451 OW 775 27.160 HOH 2.372 34.466 1.000 59.84 ATOM 2452 OW HOH 776 6.575 19.271 25.545 1.000 36.68

ATOM	2453 OW	нон	777	-17.605	29.205	62.661	1.000	56.83
ATOM	2454 OW	НОН	778	7.616	6.902	24.722		
MOTA	2455 OW	НОН	779	19.749	10.700	68.006	1.000	
MOTA	2456 W	нон	780	7.281	-5.270	50.090		50.00
ATOM	2457 W	НОН	781	-6.809	28.483	40.515	1.000	50.00
ATOM	2458 W	НОН	782	9.990	17.263	38.636	1.000	50.00
ATOM	2459 W	НОН	783	5.767	-2.331	28.939	1.000	50.00
ATOM	2460 W	НОН	784	11.694	-0.118	24.984	1.000	50.00
ATOM	2461 W	HOH	785	24.442	7.952	47.994	1.000	50.00
ATOM	2462 W	HOH	786	14.251	36.889	46.491	1.000	50.00
ATOM	2463 W	HOH	787	5.759	26.477	33.851	1.000	50.00
ATOM	2464 W	HOH	788	-11.816		40.795	1.000	50.00
ATOM	2465 W	HOH	789	-2.531 -		45.829	1.000	50.00
MOTA	2466 W	нон	790	-13.002	32.034	46.612	1.000	50.00
ATOM	2467 W	нон	791	2.230	3.555	48.985	1.000	50.00
MOTA	2468 W	HOH	792	9.397	13.464	28.121	1.000	50.00
ATOM	2469 W	HOH	793	28.257	10.442	42.781	1.000	50.00
ATOM	2470 W	НОН	794	4.652	17.944	59.241	1.000	50.00
ATOM	2471 W	HOH	795	5.977	15.287	79.554	1.000	50.00
ATOM	2472 W	HOH	796	30.501	11.852	47.616	1.000	50.00
MOTA	2473 W	нон	797	5.625	14.258	54.367	1.000	50.00
MOTA	2474 W	HOH	798	23.942	20.228	33.277	1.000	50.00
MOTA	2475 W	нон	799	10.164	14.642	58.997	1.000	50.00
MOTA	2476 W	HOH	800	7.807	31.943	52.999	1.000	50.00
ATOM	2477 W	НОН	801	-23.377	9.361	34.817	1.000	50.00
ATOM	2478 W	HOH	802	21.193	9.722	32.004	1.000	50.00
ATOM	2479 W	HOH	803	34.928	14.644	46.038	1.000	50.00
MOTA	2480 W	HOH	804	29.073	16.684	34.445	1.000	50.00
ATOM	2481 W	HOH	805	7.008	-2.049	51.872	1.000	50.00
ATOM	2482 W	HOH	806	25.363	7.860	45.531	1.000	50.00
ATOM	2483 W	HOH	_807	30.704	8.207	55.971	1.000	50.00
ATOM	2484 W	HOH	808	33.072	24.900	40.599	1.000	50.00
ATOM	2485 W	HOH	809	-15.577	19.225	63.152	1.000	50.00
ATOM	2486 W	HOH	810	6.072	18.137	23.603	1.000	50.00
ATOM	2487 W	HOH.	811	-7.214	39.940	55.639	1.000	50.00
ATOM	2488 W	HOH	812	5.509	18.517	74.919	1.000	50.00
ATOM	2489 W	HOH	813	33.845	9.908	56.672	1.000	50.00
ATOM	2490 W	НОН	814	0.421	35.779	42.931	1.000	50.00
ATOM	2491 W	HOH	815	35.282	21.705	48.656	1.000	50.00
MOTA	2492 W	HOH	816	39.344	22.173	46.871	1.000	50.00
MOTA	2493 W	НОН	817	-5.192	39.820	60.056	1.000	50.00
MOTA	2494 W	НОН	818	30.199	13.039	33.383	1.000	50.00
ATOM	2495 W	НОН	819	-4.860	36.454	61.731	1.000	50.00
ATOM	2496 W	НОН	820	-14.599	17.407	58.382	1.000	50:00
ATOM	2497 W	нон	821	1.340	-0.111	41.711	0.500	50.00
MOTA	2498 W	НОН	822	34.512	23.218	52.108	1.000	50.00
MOTA	2499 W	нон	823	32.136	12.571	52.190	1.000	50.00
ATOM	2500 W	нон	824	13.525	-6.549	29.838	1.000	50.00
MOTA	2501 W	нон	825	6.072	-4.141	27.534	1.000	

## STRUCTURE B

ATOM ANISOU ATOM A	7 N N A A B B G G G G G G G G G G G G G G G G	ASP THR THR THR THR THR THR THR THR THR THR	4 4 4	31.63.06 30.03.06 30.05.06 30.05.06 30.05.06 30.05.06 30.06	16.044 2485 17.181 2456 18.465 2426 19.650 2429	98.09 98.09 98.08 92.46 55.55 98.10 98.08 99.08 10.05 10	1.000 50.96 1113 -2217 - 554 1.000 51.63 691 -1891 169 1.000 40.50 833 -1535 - 460 1.000 45.32 -239 -653 -1702 1.000 52.14 287 -2128 - 63 1.000 52.92 1417 -4224 519 1.000 57.78 34 -1912 - 811 1.000 54.62 137 -2012 - 617 1.000 43.52 474 -2350 47 1.000 41.69 -309 -2603 - 31 1.000 37.89 -304 -3473 2 6 6 1.000 39.59 15 -3218 589 1.000 45.10 -553 -1950 - 625 1.000 42.05 -465 -3788 1 45 1.000 33.84 -59 -1682 - 122 1.000 29.25 658 -390 - 615 1.000 29.41 907 -2076 - 284 1.000 28.55 597 -1006 - 390 1.000 36.51 -791 -1996 5 2 1.000 29.41 907 -2076 - 284 1.000 28.55 597 -1006 - 390 1.000 36.51 -791 -1996 5 2 1.000 29.41 907 -2076 - 284 1.000 29.41 907 -2076 - 284 1.000 28.55 597 -1006 - 390 1.000 36.51 -791 -1996 5 2 1.000 29.01 738 -1079 9 9 1.000 35.82 390 524 -1246 1.000 24.98 542 -2040 - 986 1.000 23.97 344 -1563 - 375 1.000 26.77 651 -988 - 923
ANISOU 2 ATOM 2 ANISOU 2 ATOM 2	24 N 25 CA 25 CA 26 CB	THR THR THR THR	4 4 4	3874 26.214 3437 27.183	17.181 2456 18.465 2426 19.650	60.332 3162 60.327 3244 60.408	1.000 24.98 542 -2040 - 986 1.000 23.97 344 -1563 - 375 1.000 26.77
ATOM 2 ANISOU 2 ATOM 2 ANISOU 2 ATOM 2 ANISOU 2 ATOM 3 ANISOU 3	7 OG1 27 OG1 28 CG2 28 CG2 29 C	THR THR THR THR THR THR THR THR	4 4 4 4 4 4		2429 19.484 2812 20.942 2692 18.577 2760 18.264 2629	5105 61.551 6184 60.663 4967 59.097 2374 57.980 2902	

- 90 -

- 91 -

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ANISOU 41 CB PRO 6 2294 1740 2886 -224 130 4 3 4
ATOM 42 CG PRO 6 25.132 20.378 54.409 1.000 20.37
ANISOU 42 CG PRO 6 2708 2632 2399 -1078 38 -61
ATOM 43 C PRO 6 23.576 23.091 55.510 1.000 14.59
ANISOU 43 C PRO 6 1388 1712 2443 -406 -786 6 9 8
ATOM 44 O PRO 6 1298 1547 2118 -283 -596 1 5
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            39 CD PRO 6 24.302 19.770 55.484 1.000 15.56
 ATOM
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ATOM 46 CA THR 7
ANISOU 46 CA THR 7
ATOM 47 CB THR 7
ANISOU 47 C3 THR 7
ATOM 48 OG1 THR 7
ANISOU 48 OG1 THR 7
ANISOU 48 CG2 THR 7
ANISOU 49 CG2 THR 7
ANISOU 50 C THR 7
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3136 2013 1858 -333 -829 1 7
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CD2 PHE 8 26.006 24.882 50.079 1.000 17.52
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ATOM 55
ANISOU 55
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ATOM 94
ATOM 95
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ANISOU 97
ANISOU 97
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ATOM 99 N GLN 14 23.945 29.534 42.472 1.000 16.86 ANISOU 99 N GLN 14 1970 2337 2100 -557 -6838 ATOM 100 CA GLN 14 23.657 30.015 41.132 1.000 18.63 ANISOU 100 CA GLN 14 2761 2404 1915 -610 -802 5 ATOM 101 CB GLN 14 22.421 30.923 41.130 1.000 19.39 ANISOU 101 CB GLN 14 3166 2176 2025 -392 -918 9 ATOM 102 CG GLN 14 21.108 30.250 41.460 1.000 19.00 ANISOU 102 CG GLN 14 2879 2383 1957 -209 -725 4 ATOM 103 CD GLN 14 19.974 31.227 41.766 1.000 18.83 ANISOU 103 CD GLN 14 3139 2118 1897 -6 -1229 49 4 ATOM 104 OF1 GLN 14 20 177 32 317 42 314 1 000 26 100
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U 105 NE2 GLN 14 2900 2716 2340 -149 -840 4 5 4
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J 116 O GLN 15 3535 4619 2845 -899 510 1225  
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J 117 N GLY 16 4089 3282 2457 -889 -36 4 6 9  
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J 118 CA GLY 16 4785 3562 2671 -677 765 2 5 5  
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J 119 C GLY 16 3427 3490 2754 -264 1422 6 7 3
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ANISOU 116 0
ATOM
ANISOU 117 N
ATOM
ANISOU 118 CA GLY 16
 ATOM
ANISOU 119 C
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ATOM 120 O GLY 16

ANISOU 120 O GLY 16

ATOM 121 N LEU 17

ANISOU 121 N LEU 17

ATOM 122 CA LEU 17

ANISOU 122 CA LEU 17
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DESCRION AND ACCOUNTS

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ATOM 155 O ASP 20 31.118 19.038 47.075 1.000 20.80
ANISOU 155 O ASP 20 1162 2583 4157 -72 -139 58
ATOM 156 N GLU 21 31.359 21.177 47.729 1.000 17.88
ANISOU 156 N GLU 21 1218 2751 2824 -263 -148 58
ATOM 157 CA GLU 21 30.599 20.999 48.965 1.000 16.80
ANISOU 157 CA GLU 21 30.599 20.999 48.965 1.000 16.80
ANISOU 157 CA GLU 21 30.654 22.304 49.781 1.000 20.23
ATOM 158 CB GLU 21 30.654 22.304 49.781 1.000 20.23
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ANISOU 159 CG GLU 21 32.860 23.565 49.402 1.000 28.46
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ANISOU 163 C GLU 21 1271 2295 2679 -165 -53 4  
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ANISOU 165 N PHE 22 1440 2441 2253 -316 -28 3 3  
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ATOM 173 CE2 PHE 22 22.360 21 853 45 670

ANISOU 173 CZ PHE 22 22.360 21 853 45 670

ANISOU 173 CZ PHE 22 22.360 21 853 45 670
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ANISOU 177
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ANISOU 178
ANISOU 179
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BAG 2440
BAG 2470
BAG 258
BAG 2470
B
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CD LYS 29
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  ANISOU 242
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                                                             -56 -419 1 0 4
          244 N
  ATOM
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  ANISOU 244 N
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באובהתמות אות מחשמתיאין

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245
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                        31 19.272 17.324 52...803 1.000 11.07
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18.465 16.777 53.975 1.000 14.44
                                                      46 - 520 - 33
ATOM
        246
             CB LEU 31
                 LEU 31
ANISOU 246
                            1753 1671 2062 -284 -80 -
19.113 16.629 55.333 1.000 17.74
             СВ
                                              2062 -284 -80 -178
MOTA
        247
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ANISOU 247
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31 18.220 15.978 56.371 1.000 26.19
             CG LEU
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ATOM
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             CD1 LEU
ANISOU 248
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        249
            CD2 LEU 31 3121 2633 2899 650 -18 14 C LEU 31 20.176 18.498 53.195 1.000 10.95 C LEU 31 1041 1129 1989 180 -318 -2 O LEU 31 21.376 18.314 53.424 1.000 10.89 O LEU 31 1015 1171 1952 69 -160 2 0 4 N PHE 32 19.570 19.688 53.219 1.000 11.42 N PHE 32 1134 995 2211 75 -273 6 5 CA PHE 32 20.280 20.916 53.545 1.000 10.33
ANISOU 249
                                                      650 -18 1487
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ATOM
ANISOU 250
                                                      180 -318 - 223
        251
ATOM
ANISOU 251
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ATOM
        252 N
ANISOU 252
            N
ATOM
        253
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             CA PHE 32
CB PHE 32
ANISOU 253
                            1071
                                             1703.
                                     1152
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ATOM
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ANISOU 254
             CB PHE 32
                            1054
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                                              1872
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                 PHE 32
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ANISOU 255
             CG PHE 32
CD1 PHE 32
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CD2 PHE
                       32
                            1070
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                                             1846
                                                      -182
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1618 1353 1639 -300 -185 -
ANISOU 257
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                                                     -300 -185 - 47
ATOM
        258
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                        32
                       32 1342 1377 1840 -301 -468 3 3 2
32 19.553 22.534 49.266 1.000 12.79
32 1858 1543 1457
ANISOU 258
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             CE2 PHE
ATOM
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ANISOU 259
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19.416 21.376 48.503 1.000 11.50
ATOM
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ANISOU 260 CZ PHE 32
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                                     1414
                                             1331 -76 -272 2 1 7
ATOM 261 C
ANISOU 261 C
ATOM 262 O
ANISOU 262 O
ATOM 263 N
                           19.310 22.071 53.762 1.000 9.82
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                       32
                  PHE
                       32
                           1015
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32
33
33
33
33
                 PHE
                           18.165 21.990 53.285 1.000 11.29
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                           1097
                                     1286
                                             1906
                                                     -95 -495 - 77
                  TYR
                            19.736 23.099 54.493 1.000 12.68
ANISOU 263 N
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                            1606
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ATOM 264 CA TYR
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ANISOU 264 CA TYR
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                            1385
                                     1441
                                             1596
                                                      -68
                                                           83 - 9 4
ATOM
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ANISOU 268
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                            1879
                                     1483
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MOTA
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             CD2 TYR
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ANISOU 269
             CD2 TYR
                       33
                            1604
                                     2040
                                             1689
                                                     132
                                                            -509 1 2 7
ATOM
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        270
                        33
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ANISOU 270
             CE2 TYR
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                                     2227
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                                             1886
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                                             1942
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ATOM
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ANISOU 272 OH TYR
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                                     2154
                                             2015
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       273 C
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ATOM
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ANISOU 274
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MOTA
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                  LEU
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- 99 -ANISOU 275 N LEU 34 1159 1265 1862 -210 -149 1 2 1 18.577 26.942 51.864 1.000 12.99 276 CA LEU 34 ANISOU 276 CA LEU 34 1565 1444 81 -478 274 1926 17.757 26.420 50.682 1.000 13.96 277 CB LEU 34 ATOM ANISOU 277 CB LEU 34 1301 1995 2007 -430 -459 3 2 1 ATOM 278 CG LEU 34 17.990 27.112 49.334 1.000 13.81 ANISOU 278 CG LEU 34 2085 1322 1839 -331 -365 1 9 8 ATOM 279 CD1 LEU 34 19.308 26.691 48.704 1.000 15.94 CD1 LEU 34 ANISOU 279 2123 1793 2140 -10 -313 6 0 7 16.818 26.799 48.411 1.000 16.36 CD2 LEU 34 ATOM 280 ANISOU 280 CD2 LEU 3 4 2186 1837 2193 122 -721 1 3 4 18.195 28.361 52.241 1.000 13.03 LEU 34 281 C MOTA ANISOU 281 C 1676 1418 1857 31 -643 218 17.055 28.647 52.595 1.000 13.99 LEU 34 ATOM 282 O LEU 34 ANISOU 282 - O 1690 1690 1281 2344 140 -714 8 19.148 29.283 52.175 1.000 15.03 -714 8 5 THR 35 283 N ANISOU 283 N THR 35 1837 1584 2288 -118 -625 - 3 18.918 30.704 52.369 1.000 14.80 284 CA THR 35 ATOM ANISOU 284 CA THR 35 1866 1560 2196 -169 -175 - 144 285 CB THR 35 20.013 31.366 53.232 1.000 15.65 MOTA CB THR 35
CB THR 35
OG1 THR 35
OG1 THR 35
CG2 THR 35
CG2 THR 35
C THR 35
C THR 35 ANISOU 285 1719 2202 2025 -149 -204 -28121.276 31.115 52.601 1.000 18.81 286 ANISOU 286 1885 2679 2583 -279 -229 -20.138 30.811 54.622 1.000 18.84 -279 -229 - 728 287 MOTA ANISOU 287 2523 2207 2427 -850 -510 1 18.915 31.456 51.043 1.000 15.07 -850 -510 1 5 5 MOTA 288 1904 1473 2348 -57 -283 -19.209 30.909 49.973 1.000 15.00 2034 1520 2146 ANISOU 288 -283 - 70 THR 35 289 . 0 THR 35 2034 ANISOU 289 O 1520 2145 -215 -372 8 9 18.564 32.739 51.086 1.000 17.46 2302 1366 2968 -209 -766 -290 N ASP 36 ATOM ANISOU 290 N ASP 36 2302 -209 -766 - 120 ATOM 291 CA ASP 36 18.618 33.606 49.924 1.000 17.91 CA ASP 36 2150 1592 3063 112 -660 8 6
CB ASP 36 20.063 33.845 49.471 1.000 17.91
CB ASP 36 2153 1584 3067 84 -587 - 42
CG ASP 36 20.948 34.545 50.469 1.000 19.23
CG ASP 36 2575 2160 2571 -642 -324 18
OD1 ASP 36 20.426 35.304 51.325 1.000 24.17 ANISOU 291 112 -660 8 6 292 ATOM ANISOU 292 ATOM 293 2575 2160 2571 -642 -324 1 8 1 20.426 35.304 51.325 1.000 24.17 ANISOU 293 294 ATOM OD1 ASP ANISOU 294 36 2843 3055 3284 152 -1013 -652 22.199 34.355 50.412 1.000 21.00 OD2 ASP 36 295 ANISOU 295 OD2 ASP 36 2637 2571 2772 -382 -834 -1 17.783 33.038 48.784 1.000 18.20 2772 -382 -834 - 393 ATOM ASP 36 296 C ANISOU 296 C ASP 36 2402 1736 2779 -446 -390 1 9 1 ATOM 297 0 ASP 36 18.222 33.063 47.629 1.000 18.98 ANISOU 297 N ASP 36 2127 CYS 37 16.593 2022 3062 -464 -60 -252 ATOM 298 16.593 32.547 49.077 1.000 17.22 N CYS 37
N CYS 37
CA CYS 37
CA CYS 37
CB CYS 37
CB CYS 37
SG CYS 37 ANISOU 298 1873 2190 2479 63 - 350 - 1 MOTA 299 15.730 31.945 48.043 1.000 15.98 ANISOU 299 1997 1590 2485 -81 -65 -184 MOTA 300 15.621 30.423 48.252 1.000 18.87 ANISOU 300 2112 1790 3268 -114 -405 5 14.753 29.917 49.759 1.000 19.42 2112 -114 -405 5 7 0 ATOM 301 2532 1683 3164 -74 -230 3 14.349 32.580 47.958 1.000 16.12 ANISOU 301 -74 -230 3 2 2 MOTA CYS 37 302 С ANISOU 302 C CYS 37 19,92 1669 2465 -175 -504 1 6

2761

1847

13.483 32.032 47.253 1.000 20.60

14.125 33.714 48.617 1.000 17.89

3296

3381

12.850 34.404 48.587 1.000 18.16 1608 2126 3164 141 -999 - 6

-241 -1333 5 1

209 -898 - 111

1769

1572

303 0

304 N

N

CA

ANISOU 303 O

305

ANISOU 304

ANISOU 305

CYS 37

GLY 38

GLY 38

37

3.8

CYS

GLY

CA GLY 38

MOTA

MOTA

ATOM

DESCRIPTION ASSESSMENT I

- 100 -GLY 38 11.843 33.864 49.589 1.000 21.98 GLY 38 2598 2574 3180 262 -97 -ATOM 306 C ANISOU 306 C 262 -97 -455 38 38 39 307 0 ATOM  $\operatorname{\mathsf{GL}} \operatorname{\mathsf{Y}}$ 10.677 34.273 49.499 1.000 22.75 ANISOU 307 0 GLY 2542 3027 3073 241 79 - 97 308 N MOTA LEU 39 12.241 32.982 50.501 1.000 21.93 3 9 ANISOU 308 N LEU 2112 3318 2903 -65 -102 - 154 ATOM 39 309 CA LEU 11.443 32.357 51.545 1.000 26.16 ANISOU 309 39 CA LEU 3141 3610 3188 -1071 162 -400 MOTA 310 CB LEU 39 11.220 30.868 51.277 1.000 28.13 ANISOU 310 CB LEU 39 2980 3192 4516 -352 -848 2 5 8 ATOM 311 CG LEU 30.434 50.157 1.000 27.39 39 10.296 ANISOU 311 CG LEU 39 3352 2591 4463 541 -637 -1052 CD1 LEU ATOM 312 10.472 28.940 49.910 1.000 28.66 39 ANISOU 312 CD1 LEU 3 9 3375 2293 5221 581 -150 - 190 39 39 39 CD2 LEU ATOM 313 30.768 50.478 1.000 30.62 8.838 ANISOU 313 CD2 LEU 3155 2985 5496 1275 -1485 -208 ATOM 314 С 12.060 32.430 52.949 1.000 26.26 LEU 39 ANISOU 314 C LEU 2868 3969 3143 -796 170 3 3 5 ATOM 315 0 13.105 31.861 53.266 1.000 35.57 LEU 39 3 9 4 0 ANISOU 315 O 
 4990
 4057
 4470
 804
 -6303

 11.388
 33.136
 53.827
 1.000 26.61
 LEU 804 -630 3 2 0 ATOM 316 N THR ANISOU 316 N 40 ANISOU 310 N THE ATOM 317 CA THR ANISOU 317 CA THR ATOM 318 C THR ANISOU 318 C THR ATOM 319 O THR ANISOU 319 O THR ATOM 320 CB THR ANISOU 320 CB THR ANISOU 321 CG1 THR THR 3425 3883 2803 -703 -191 1 0 2 40 3425 3883 2803 -703 -191 1 40 11.676 33.329 55.228 1.000 22.95 40 1972 3864 2886 4 -603 518 THR 40 10.380 33.424 56.031 1.000 27.03 THR 40 2331 4900 3040 -690 -220 - 3THR 40 9.254 33.316 55.537 1.000 25.98 THR 40 2148 4860 2864 -546 36 - 72
THR 40 12.476 34.624 55.456 1.000 27.16 -546 36 - 720 4 0 4 0 4 0 2646 4799 2874 -932 -391 1 4 8 OG1 THR ATOM 321 11.639 35.687 54.986 1.000 36.24 OG1 THR ANISOU 321 5158 3872 4740 -472 -136 6 6 0 CG2 THR 40 ATOM 322 13.771 34.669 54.659 1.000 34.29 ANISOU 322 CG2 THR 40 5268 3289 4470 -1303 2206 4 2 9 ATOM 323 N ASP 41 10.524 33.635 57.346 1.000 28.20 ANISOU 323 N ASP 41 2270 ANISOU 323 N ASP ATOM 324 CA ASP ANISOU 324 CA ASP ATOM 325 C ASP ANISOU 325 C ASP ATOM 326 O ASP ANISOU 326 O ASP ANISOU 327 CB ASP ANISOU 327 CB ASP ANISOU 327 CB ASP 5223 3223 -711 -317 -479 33.604 58.191 1.000 25.10 41 9.324 41 1935 4633 2968 13 -551 -505 41 8.418 34.785 57.896 1.000 24.69 41 2686 3839 2855 -446 -749 -24141 7.219 34.846 58.163 1.000 24.79 41 2757 2721 3941 174 -584 - 141 41 9.728 41 2221 41 9.892 41 6437 33.549 59.678 1.000 28.21 5503 2995 892 -594 - 555 328 CG ASP ATOM 32.129 60.180 1.000 42.46 ANISOU 328 CG ASP 5911 3784 -1196 -1257 31.161 59.401 1.000 55.96 -1196 -1257 8 2 6 ATOM 41 9.705 329 OD1 ASP ANISOU 329 OD1 ASP 12184 41 5138 3940 -2654 -82 1249 31.951 61.383 1.000 61.55 ATOM 330 OD2 ASP 41 10.214 ANISOU 330 OD2 ASP 41 10370 7470 -4396 -4720 2309 5548 ATOM 331 N THR 35.807 57.305 1.000 29.30 42 8.991 N ANISOU 331 THR 42 3761 4531 2839 -1404 - 1089 - 72CA THR CA THR C THR MOTA 332 42 8.255 36.976 56.863 1.000 33.69 ANISOU 332 42 4852 3472 4475 -1524 - 819 - 127ATOM 333 42 7.199 36.598 55.834 1.000 29.14 ANISOU 333 C THR 42 3354 3051 -648 - 277 4667 204 0 ATOM 334 THR 42 6.026 36.969 55.844 1.000 36.90 ANISOU 334 0 THR 42 3578 2980 7462 603 -176 6 4 3 ATOM 335 СB THR 42 9.282 37.967 56.281 1.000 40.80 ANISOU 335 CB THR 42 5831 4318 5354 -2254 -450 3 7 ATOM 336 OG1 THR 42 10.288 38.317 57.263 1.000 46.30

		- 101 -	
ANISOU 345 OE1 ATOM 346 OE2 ANISOU 346 OE2 ATOM 347 N ANISOU 347 N ATOM 348 CA ANISOU 348 CA ANISOU 349 CB ANISOU 349 CB ATOM 350 CG ANISOU 350 CG ANISOU 351 CD1 ANISOU 352 CD2	THR 42 8.582	3682 6912 39.253 55.872 3877 4363 35.773 54.862 4360 4319 35.355 53.810 4683 3913 34.324 54.330 3297 4363 34.138 53.764 2970 7717 34.811 52.608 6532 3779 35.745 52.010 7105 53.77 35.764 52.826 7977 35.764 52.826 7977 35.764 52.826 7977 35.080 82.433 8930 8050 33.645 55.426 2161 3964 32.592 55.959 1973 4187 31.585 56.727 35.080 \$2.433 8930 8050 33.645 55.426 2161 3964 32.592 55.959 1973 4187 31.585 56.727 2194 33448 30.494 57.533 2801 3398 29.535 56.656 2239 4514 29.703 58.361 2869 4080 33.145 56.841 3182 4800 33.145 56.841 3182 4800 33.145 56.867 3299 3768 34.247 57.547 2938 5083 34.751 58.623 2817 4761 35.014 58.195	1.000 35.40 -1510 -860 3 2 9 1.000 28.03 -41 -919 1 6 8 1.000 38.18 -66 -2774 1 4 6 9 1.000 38.89 -2546 -860 - 3 9 3 1.000 45.47 -2936 -92 - 2 8 9 1.000 46.40 -3155 548 - 1 2 1 0 1.000 55.20 -2062 -1002 - 6 6 9 1.000 56.77 -2652 939 - 1 2 5 8 1.000 22.72 464 -476 - 4 5 0 1.000 26.76 140 570 - 9 8 6 1.000 28.25 -153 277 - 5 6 2 1.000 32.03 -279 1192 - 6 2 7 1.000 37.95 -1148 2039 - 1 4 0 3 1.000 36.97 1150 2171 1 8 6 1.000 37.95 -1148 2039 - 1 4 0 3 1.000 36.97 1150 2171 1 8 6 1.000 37.95 -1148 2039 - 1 4 0 3 1.000 36.97 1150 2171 1 8 6 1.000 37.95 -1148 2039 - 1 4 0 3 1.000 36.97 1150 2171 1 8 6 1.000 27.09 -751 467 - 2 1 40 1.000 24.95 -784 709 - 1 2 5 7 1.000 22.50 -784 709 - 1 2 5 7 1.000 24.95 -784 709 - 1 2 5 7 1.000 24.95 -784 709 - 1 2 5 7 1.000 25.85 -784 709 - 1 2 5 7 1.000 26.85 -1732 618 - 1 1 8 4 1.000 24.97 -1223 511 - 1 1 0 5 1.000 32.35 -2232 70 - 4 5 8
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367
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MOTA
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ATOM
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               LYS
                    48
ANISOU 374
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               LYS
                    48
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MOTA
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           CB LYS 48
ANISOU 375
           CВ
               LYS 48 2400
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ATOM
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           CG
               LYS 48 1.237
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ANISOU 376
           CG
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               LYS 48
LYS 48
LYS 48
LYS 48
LYS 48
ATOM
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ANISOU 377
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ATOM
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MOTA
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MOTA
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ANISOU 382
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ATOM
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ANISOU 383
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49
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ATOM
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ANISOU 384
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ATOM
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ANISOU 386
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ATOM
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               ASP 49
ANISOU 387
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ATOM
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                       -15.983 24.732 48.954 1.000 18.77
ANISOU 517 O
               ALA
                   65
                       1830
                              2178
                                     3123
                                            122
                                                 -8 - 2 2 9
ATOM
      518 N
               VAL
                   66
                       -15.100 24.248 50.973 1.000 17.99
ANISOU 518
          N
               VAL
                   66
                       1547
                              2151
                                     3137
                                            -86
                                                  36 - 196
ATOM
      519
           CA
              VAL
                   66 -13.746 24.066 50.430 1.000 16.74
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- 107 -ANISOU 519 CA VAL 66 1553 1859 2948 -62 -56 -254 CB VAL 66 -12.775 25.151 50.951 1.000 17.29 ATOM 520 520 CB VAL 66 -12.775 25.151 50.951 1.000 17.29
520 CB VAL 66 1805 1804 2963 -330 338 -185
521 CG1 VAL 66 -13.238 26.532 50.455 1.000 16.70
521 CG1 VAL 66 1547 1800 2997 111 545 -553
522 CG2 VAL 66 -12.652 25.180 52.462 1.000 18.65
522 CG2 VAL 66 2053 1996 3036 -193 17 -538
523 C VAL 66 -13.201 22.680 50.724 1.000 15.66
523 C VAL 66 1775 1813 2362 -70 -250 - 457
524 O VAL 66 -11.972 22.493 50.808 1.000 14.19
524 O VAL 66 1747 1576 2069 -122 -56 -347
525 N THR 67 -14.071 21.695 50.873 1.000 14.46
526 CA THR 67 1350 1602 2343 126 -48 -722
526 CA THR 67 1461 1698 2185 234 5 -740 ANISOU 520 ATOM 521 ANISOU 521 ATOM ANISOU 522 MOTA ANISOU 523 ATOM 524 ANISOU 524 O ATOM ANISOU 525 N ATOM ANISOU 526 CA THR 67 1461 1698 2185 234 5 -740 ATOM 527 CB THR 67 -14.419 19.647 52.225 1.000 15.08 ANISOU 527 CB THR 67 1721 1955 2053 -51 -426 - 444 ATOM 528 OG1 THR 67 -14.089 20.337 53.453 1.000 17.41 OG1 THR 67 2538 1949 2128 -39 70 -716 ANISOU 528 ANISOU 528 OG1 THR 67 2538 1949 2128 -39 70 -716
ATOM 529 CG2 THR 67 -13.915 18.215 52.420 1.000 16.63
ANISOU 529 CG2 THR 67 2182 1888 2248 148 293 -658
ATOM 530 C THR 67 -14.067 19.518 49.728 1.000 12.37
ANISOU 530 C THR 67 1144 1422 2132 209 -95 -517
ATOM 531 O THR 67 -15.208 19.567 49.229 1.000 14.82
ANISOU 531 O THR 67 1197 2086 2350 208 -168 -362
ATOM 532 N SER 68 -13.092 18.790 49.180 1.000 11.61
ANISOU 532 N SER 68 1109 1421 1881 37 -58 -534
ATOM 533 CA SER 68 -13.306 17.955 48.003 1.000 11.45
ANISOU 533 CA SER 68 1274 1444 1631 -49 -30 -374
ATOM 534 CB SER 68 -12.027 17.317 47.480 1.000 11.88 ANISOU 533 CA SER 68 1274 1444 1631 -49 -30 -374
ATOM 534 CB SER 68 -12.027 17.317 47.480 1.000 11.88
ANISOU 534 CB SER 68 1446 1523 1544 79 252 -157
ATOM 535 OG SER 68 -11.026 18.292 47.239 1.000 16.95
ANISOU 535 OG SER 68 1557 2314 2569 -336 389 -218
ATOM 536 C SER 68 -14.269 16.815 48.319 1.000 11.56
ANISOU 536 C SER 68 1287 1375 1732 -61 53 -406
ATOM 537 O SER 68 1287 1375 1732 -61 53 -406
ATOM 537 O SER 68 1998 1860 1697 -538 153 -430
ATOM 538 N PRO 69 -15.026 16.324 47.344 1.000 12.78
ANISOU 538 N PRO 69 1476 1473 1905 -243 -88 -194
ATOM 539 CD PRO 69 -15.130 16.801 45.953 1.000 12.47
ANISOU 539 CD PRO 69 -15.130 16.801 45.953 1.000 12.47
ANISOU 539 CD PRO 69 -15.941 15.214 47.639 1.000 12.21
ANISOU 540 CA PRO 69 1358 1369 1913 -178 148 -437 ANISOU 540 CA PRO 69 1358 1369 1913 -178 148 -437 ATOM 541 CB PRO 69 -16.825 15.193 46.355 1.000 13.94 ATOM 541 CB PRO 69 -16.825 15.193 46.355 1.000 13.94

ANISOU 541 CB PRO 69 1362 1591 2343 -251 -178 - 14

ATOM 542 CG PRO 69 -15.924 15.715 45.290 1.000 14.38

ANISOU 542 CG PRO 69 1396 1947 2122 -554 -511 1 78

ATOM 543 C PRO 69 -15.270 13.882 47.912 1.000 13.25

ANISOU 543 C PRO 69 1206 1526 2303 -217 -115 -100

ATOM 544 O PRO 69 -15.932 12.985 48.481 1.000 14.01

ANISOU 544 O PRO 69 1753 1450 2122 -373 99 -301

ATOM 545 N VAL 70 -14.015 13.692 47.554 1.000 13.46

ANISOU 545 N VAL 70 -13.184 12.548 47.898 1.000 13.49 -217 -115 -100 U 545 N VAL 70 1288 1479 2348 -174 -108 -546 CA VAL 70 -13.184 12.548 47.898 1.000 13.49 U 546 CA VAL 70 1404 12.548 -174 -108 - 265 ATOM ANISOU 546 CA VAL 70 1404 1692 2030 37 138 - 195 CB VAL 70 -12.587 11.720 46.737 1.000 16.39 ATOM 547 ANISOU 547 CB VAL 70 2142 1648 2439 -225 614 -4 CG1 VAL 70 -13.615 10.756 46.208 1.000 33.50 -225 614 -452 ATOM 548 ANISOU 548 CG1 VAL 70 6470 2984 3274 -2702 41 -867 ATOM 549 CG2 VAL 70 -11.995 12.613 45.640 1.000 16.46 ANISOU 549 CG2 VAL 70 1749 2234 2273 269 444 2 70 1749 2234 2273 269 444 2 3

- 108 -

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ANISOU 550
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                                                      -114 1 2 7
MOTA
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                     70
                VAL
                         -11.426 14.105 48.493 1.000 14.20
ANISOU 551
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                VAL
                     70
                         1743
                                        1964
                                 1685
                                                -265 26 182
MOTA
       552
           N
                PRO
                     71
                         -11.786 12.365 49.898 1.000 14.21
ANISOU 552
           N
                PRO
                    71
                         1607
                                 1507
                                        2285
                                                -115 -62 310
                         -12.432 11.125 50.378 1.000 14.70
MOTA
       553
           CD
               PRO
                    71
ANISOU 553
           CD
               PRO
                    71
                         1920
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                                        2076
                                                -201 646 4
                         -10.830 12.919 50.878 1.000 17.41
ATOM
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ANISOU 554
            CA
               PRO
                    71
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MOTA
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                PRO
                    71
                         -11.338 12.304 52.193 1.000 20.87
ANISOU 555
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                         3768
                                 2082
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                                                -743
                                                     190 1 4
MOTA
       556
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            CG
                PRO
                     71
ANISOU 556
           -CG
               PRO
                     71
                         3534
                                1665
                                        1746
                                                -338 781 -54
ATOM
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           С
                PRO
                     71
                        -9.384 12.543 50.619 1.000 17.14
ANISOU 557
           С
                PRO
                    71
                         2183
                                2304
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                                        2026
ATOM
       558
                    71
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                PRO
                         -8.730
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ANISOU 558
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                PRO
                    71
                         2745
                                2610
                                        2448
                                               -87
                                                     -404 4 1 4
ATOM
       559
           Ν
                THR
                    72
                        -8.834
                                13.111 49.556 1.000 16.59
ANISOU 559
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                THR
                    72
                        2156
                                2046
                                        2103
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ATOM
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           CA
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                        -7.496
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                    72
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                                1884
                                        2626
                                                -254 -510 -288
ATOM
       561
           CB
                THR
                    72
                        -7.477
                                12.829 47.545 1.000 15.98
ANISOU 561
            CB
                THR
                    72
                        1700
                                1761
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                                                    -458 - 421
           OG1 THR
ATOM
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                        -8.027
                                14.094 47.128 1.000 17.28
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                                               27 - 355 - 271
ATOM
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                       1296
           CG2 THR
ANISOU 563
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                                1581
                                        1923
                                               -46
                                                     328 - 127
ATOM
       564 C
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                    72
                        -6.418
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ANISOU 564 C
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                                               -155 -1228 2 3 2
ATOM
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               THR
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                                2265
                                        3257
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ATOM
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               MET
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ANISOU 567
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MOTA
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ATOM
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                    73
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                                15.059 52.843 1.000 27.01
ANISOU 569
           CG
               MET
                    73
                        3545
                                2853
                                        3864
                                               -84
                                                     -87 1526
ATOM
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               MET
                    73
                        -4.107
                                14.850 54.107 1.000 32.23
ANISOU 570
           SD
               MET
                    73
                        4364
                                4245
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                                               469
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ATOM
       571
           CE
               MET
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                    73
                                13.492 53.374 1.000 26.74
ANISOU 571
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                                4895
                                        2381
                                               326
                                                     425 1348
MOTA
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               MET
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ATOM
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                        1881
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ATOM
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ANISOU 575
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               ARG
                    74
                        937 1986
                                     3053
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ATOM
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          CB
               ARG
                    74
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ANISOU 576
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               ARG
                    74
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MOTA
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                    74
           CG
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ANISOU 577
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MOTA
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               ARG
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                        1967
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                                               268
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MOTA
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               ARG
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ATOM
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- 109 -ANISOU 580 CZ ARG 74 1968 1646 2709 -141 -190 - 596 NH1 ARG 74 -5.951 18.775 41.293 1.000 20.09 ATOM 581 74 1899 ANISOU 581 NH1 ARG 2075 3660 54 - 353 - 788 74 -4.220 17.896 40.068 1.000 20.12 582 NH2 ARG ANISOU 582 NH2 ARG 74 2366 2844 2437 153 -196 - 400 ATOM 583 C ARG 74 -5.373 18.681 46.966 1.000 12.70 ANISOU 583 C 74 1187 ARG 1880 1758 6 -22 -136 ATOM 584 O 74 -4.501 19.465 46.582 1.000 14.07 ARG ANISOU 584 O ARG 74 1049 2048 2247 -221 -170 - 480 ATOM 585 N ARG 75 -6.567 19.099 47.387 1.000 12.72 ANISOU 585 N 75 1402 ARG 1702 1728 95 182 - 108 ATOM 586 CA ARG ANISOU 586 CA ARG ATOM 587 CB ARG 75 -7.006 20.471 47.308 1.000 13.40 1924 1618 1548 87 275 - 193 -7.737 20.784 45.995 1.000 13.45 75 75 75 1972 1387 1751 -179 51 - 9 75 -6.908 20.637 44.721 1.000 13.38 ANISOU 587 CB ARG ATOM 588 CG ARG ANISOU 588 CG AFG 75 1638 75 1638 1851 1594 78 -217 101 75 -5.849 21.708 44.582 1.00012.85 78 -217 101 589 CD AKG ATOM ANISOU 589 CD ARG 75 1537 ANISOU 589 CD ARG 75 1537 1602 1741 237 62 - 15 ATOM 590 NE ARG 75 -5.087 21.685 43.347 1.000 13.71 1602 ANISOU 590 NE ARG 75 1708 1797 1705 188 90 - 91 591 CZ 591 CZ ATOM 75 -3.984 21.036 43.013 1.000 12.46 ARG ANISOU 591 ARG 75 1348 1656 1731 -89 86 1 1 7 ATOM 592 NH1 ARG  $75 \quad -3.418 \quad 20.241 \quad 43.894 \quad 1.000 \quad 14.64$ NH1 ARG ANISOU 592 75 1933 1794 1834 186 -91 6 5 593 NH2 ARG ATOM 75 -3.444 21.167 41.794 1.000 13.72 ANISOU 593 NH2 ARG 75 1510 2037 1667 -136 84 - 83 -7.948 20.787 48.475 1.000 12.74 ATOM 594 C 75 ARG ANISOU 594 C 75 1400 1656 1784 -209 214 -4 75 -8.780 19.944 48.818 1.000 14.60 75 1400 ARG -209 214 -464 595 O ARG ATOM ANISOU 595 O ARG 75 1348 1926 2273 -427 156 -480 76 -7.830 21.955 49.078 1.000 11.92 ATOM 596 N GLY ANISOU 596 N  $\operatorname{\mathsf{GL}} \mathtt{Y}$ 76 1268 1537 1724 -22 34 - 389ATOM 597 CA GLY 76 -8.801 22.395 50.070 1.000 12.44 ANISOU 597 CA GLY 76 1439 1493 1796 -315 263 -412 ATOM 598 C ANISOU 598 C ATOM 599 O ANISOU 599 O GLY 76 -8.536 21.857 51.469 1.000 12.50 76 1324 GLY1527 1900 5 326 - 273 76 -7.388 21.517 51.769 1.000 14.25 76 1100 2099 2218 -277 239 -225 77 -9.574 21.840 52.287 1.000 12.65 77 1191 1806 1809 -162 231 -351 77 -9.526 21.474 53.694 1.000 14.00 GLY GLY ATOM 600 N PHEANISOU 600 N PHE ATOM 601 CA PHE 77 1295 2110 1914 -260 276 -77 -10.644 22.226 54.451 1.000 14.73 ANISOU 601 CA PHE -260 276 -138 602 CB PHE ATOM ANISOU 602 CB PHE 77 1554 2169 1874 -402 485 -77 -10.773 21.824 55.912 1.000 17.13 -402 485 -317 ATOM 603 CG PHE ANISOU 603 CG PHE 77 1927 2730 1849 -374 378 -243ATOM 604 CD1 PHE 77 -9.949 22.369 56.886 1.000 19.49 ANISOU 604 CD1 PHE 77 2744 2700 1962 -119 219 -789 ATOM 605 CD2 PHE 77 -11.730 20.902 56.309 1.000 19.13 CD2 PHE ANISOU 605 2348 77 3068 1852 -501 864 - 165 ATOM 606 CE1 PHE 77 -10.068 21.973 58.217 1.000 19.75 ANISOU 606 CE1 PHE 77 2956 2381 2168 -174 -313 -304ATOM 607 CE2 PHE 77 -11.829 20.479 57.627 1.000 18.73 ANISOU 607 CE2 PHE 77 2565 2711 1841 -382 310 -77608 CZ PHE MOTA 77 -10.986 21.013 58.584 1.000 19.22 ANISOU 608 CZ PHE 77 2378 2542 2382 98 13 - 364 MOTA 609 C PHE 77 -9.668 19.976 53.924 1.000 13.73 77 1306 ANISOU 609 C PHE 2096 1813 -368 21 - 204 77 -10.520 19.313 53.291 1.000 16.02 77 1386 2508 2194 -470 -128 -MOTA 610 O PHE ANISOU 610 O PHE -470 -128 - 425

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        612
             CA
                 THR
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 ANISOU 612
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                 THR
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                          1813
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 MOTA
        613
             CВ
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ANISOU 613
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                 THR
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                 THR
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ATOM
        617
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ANISOU 617
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                 THR
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ATOM
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ANISOU 618
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                 GLY
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                                                 -1352 19 4 5
ATOM
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ANISOU 619
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MOTA
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                 GLY
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ANISOU 622
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2848 2777 3904 206 621 3
                LEU
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ANISOU 623
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ATOM
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ANISOU 624
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ATOM
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ANISOU 625
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ANISOU 626
            СВ
                LEU
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ATOM
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ANISOU 627
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MOTA
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ANISOU 628
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ATOM
            CD2 LEU
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ANISOU 629
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ATOM
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ANISOU 630
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MOTA
       631 CA
                GLU
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ANISOU 631
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                GLU
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ATOM
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ANISOU 632
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ATOM
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ANISOU 634
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ATOM
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ANISOU 635
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ATOM
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ANISOU 637
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ANISOU 638
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ATOM
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ANISOU ATOM ANISOU ANI	$\begin{array}{c} 4444444444444444445555555555555555555$	CB CB CCD1 CD2 CD2 CE1 CE2 CE2	RRRRRRRRYYYYYYYYYYYYYYRRRRRRRRRRRRRRRR	999999999999999999999999999999999999999	3 4 3 3 3 3 4 6 3 3 3 4 6 3 3 6 4 3 5 3 6 4 3 6 7 6 6 6 6 6 6 6 6 6 6 6 6 6 6 6 6 6	75992 11.674558 11.474558 11.5904412 11.5904412 11.5904413 11.5046666 11.50466666 11.50466666 11.50466666 11.504666666 11.504666666 11.504666666 11.504666666 11.504666666 11.504666666 11.504666666 11.504666666 11.504666666 11.5046666666 11.504666666 11.5046666666 11.5046666666 11.5046666666 11.5046666666 11.5046666666 11.5046666666 11.5046666666 11.5046666666 11.5046666666 11.50466666666 11.5046666666 11.50466666666 11.5046666666 11.50466666666 11.50466666666 11.50466666666 11.50466666666 11.50466666666 11.50466666666 11.50466666666 11.50466666666 11.50466666666 11.504666666666 11.504666666666 11.504666666666 11.504666666666 11.504666666666 11.504666666666 11.504666666666 11.504666666666 11.504666666666 11.504666666666 11.504666666666 11.504666666666 11.50466666666666 11.504666666666 11.504666666666 11.504666666666 11.504666666666 11.504666666666 11.504666666666 11.50466666666 11.504666666666 11.50466666666 11.50466666666 11.50466666666 11.50466666666 11.50466666666 11.50466666666 11.5046666666 11.5046666666 11.5046666666 11.5046666666 11.5046666666 11.5046666666 11.504666666 11.504666666 11.504666666 11.504666666 11.504666666 11.504666666 11.504666666 11.504666666 11.504666666 11.504666666 11.504666666 11.50466666 11.504666666 11.504666666 11.504666666 11.50466666 11.50466666 11.50466666 11.50466666 11.50466666 11.50466666 11.50466666 11.50466666 11.50466666 11.50466666 11.50466666 11.50466666 11.50466666 11.50466666 11.50466666 11.50466666 11.50466666 11.504666666 11.50466666 11.50466666 11.5046666 11.5046666 11.5046666 11.5046666 11.5046666 11.5046666 11.5046666 11.5046666 11.5046666 11.5046666 11.5046666 11.5046666 11.5046666 11.5046666 11.504666 11.5046666 11.5046666 11.5046666 11.5046666 11.504666 11.5046666 11.5046666 11.5046666 11.5046666 11.5046666 11.5046666 11.5046666 11.5046666 11.5046666 11.50466666 11.5046666 11.5046666 11.5046666 11.5046666 11.5046666 1	48.3.3.5.4.6.6.8.7.7.4.0.8.7.7.4.0.8.7.7.4.0.8.7.7.4.0.8.7.7.4.0.8.7.7.4.0.8.7.7.4.0.8.7.7.4.2.0.4.0.8.7.7.4.2.0.4.0.8.7.7.4.2.0.4.0.8.7.7.4.2.0.8.7.7.4.2.0.8.7.7.4.2.2.6.3.1.4.3.8.8.0.8.8.0.1.4.3.8.8.0.8.8.7.5.4.3.8.8.0.8.8.7.5.4.3.8.8.0.8.8.7.5.4.3.8.8.0.8.8.7.7.8.8.8.0.8.8.7.7.8.8.8.0.8.8.9.4.9.8.8.0.8.8.7.7.8.8.0.8.8.0.8.9.4.9.8.8.0.8.0.8.8.0.8.8.0.8.8.0.8.8.0.8.8.0.8.8.0.8.8.0.8.8.0.8.0.8.0.8.0.8.0.8.8.0.8.0.8.0.8.0.8.0.8.0.8.0.8.0.8.0.8.0.8.0.8.0.0.8.0.8.0.8.0.0.8.0.8.0.0.8.0.0.8.0.0.8.0.0.8.0.0.8.0.0.0.8.0	-102 -1104 8 4 7 1.000 34.01 458 -1188 1 3 4 1.000 34.74 -232 -979 9 7 1 1.000 41.53 236 -1958 9 7 0 1.000 42.64 -2166 2340 - 4 2 7 1.000 44.91 -4311 -1561 5 6 5 1.000 38.67 -2821 -274 - 1 5 9 1.000 32.45 -183 1152 - 4 3 9 1.000 31.97 -1382 735 - 5 7 1 1.000 33.02 -1716 851 - 9 5 6 1.000 26.22 -885 741 - 9 4 7 1.000 23.91 -680 548 - 5 6 7 1.000 23.77 -372 736 - 5 6 0 1.000 23.41 -386 970 - 3 9 9 1.000 24.26 -286 833 - 2 2 4 1.000 27.06 630 92 - 3 8 6 1.000 25.71 -576 271 - 5 0 6 1.000 28.14 -373 290 5 1 7 1.000 24.24 -204 791 - 8 1 7 1.000 23.94 95 1112 - 6 8 3 1.000 25.19 147 737 - 6 2 5 1.000 23.94 95 1112 - 6 8 3 1.000 25.19 147 737 - 6 2 5 1.000 23.94 95 1112 - 6 8 3 1.000 25.19 147 737 - 6 2 5 1.000 23.94 95 1331 - 5 2 5 1.000 23.94 95 1312 - 6 8 3 1.000 25.19 147 737 - 6 2 5 1.000 23.94 95 1312 - 6 8 3 1.000 25.19 147 737 - 6 2 5 1.000 23.94 95 134 - 2 7 4 1.000 26.01 499 353 - 5 4 3 1.000 27.06
ANISOU ATOM ANISOU ATOM ANISOU ATOM ANISOU	667 668 669 669 670	CE1 CE2 CE2 CZ CZ OH OH	TYR TYR TYR TYR TYR TYR TYR	9 4 9 4 9 4	4559 -12.375 4707 -13.209 5641 -14.059 3079	3328 9.159 2585 9.247 3518 8.281 3962	3037 61.305 2764	434 140 -1370 1.000 26.47 -220 1227 -718
ATOM ANISOU	671 671	N N	SER SER	95 95	-10.628 2460	15.714 2497	62.561 3632	1.000 22.61 -54 59 - 338

- 112 -CA SER 95 ATOM 672 -9.924 16.975 62.750 1.000 22.54 ANISOU 672 CA SER 95 2257 2603 3706 -120 -301 4 6 -9.370 17.106 64.163 1.000 23.58 ATOM 673 C SER 95 ANISOU 673 C SER 95 1811 3478 3671 -521 -88 -85 -8.623 18.034 64.481 1.000 26.53 MOTA 674 0 SER 95 ANISOU 674 O 95 SER 2592 3242 4247 -469 -167 -641 СВ ATOM -10.838 18.177 62.478 1.000 27.58 675 SER 95 CB OG ANISOU 675 SER 95 3657 2556 4264 365 -379 2 8 ATOM 95 -11.506 18.093 61.242 1.000 39.40 676 SER ANISOU 676 OG 9 5 SER 6336 4214 4421 900 -1445 1442 677 N ATOM -9.712 16.194 65.060 1.000 25.04 ASP 96 ANISOU 677 N ASP 96 2579 3688 3248 -399 277 -232 678 CA ASP ATOM 96 -9.228 16.317 66.422 1.000 24.42 ANISOU 678 CA ASP 96 2603 3347 3330 -470 257 -526 ATOM 679 C ASP 96 16.050 66.501 1.000 24.45 -7.735 ANISOU 679 C 96 ASP 2597 3228 3466 -471 162 -383ATOM 680 O ASP 96 -7.073 16.589 67.404 1.000 26.51 ANISOU 680 O ASP ATOM 681 CB ASP 96 2656 4047 3370 -170 160 - 798 -9.952 15.334 67.334 1.000 24.97 96 ANISOU 681 CB ASP 96 2310 3806 3371 -423 -228 7 7 CG CG ATOM 682 ASP 96 -11.411 15.605 67.606 1.000 26.77 ANISOU 682 ASP 96 2272 4334 3566 -362 -240 7 1 6 OD1 ASP ATOM 683 -11.935 16.723 67.388 1.000 33.94 96 ANISOU 683 OD1 ASP 96 3267 4894 4733 647 204 569 ATOM 684 OD2 ASP -12.058 14.646 68.083 1.000 32.65 96 ANISOU 684 OD2 ASP 96 3624 4709 4072 -1032 1446 - 202 MOTA 685 N TYR 97 15.226 65.581 1.000 22.21 -7.254 ANISOU 685 N TYR 97 2292 3389 2760 -376 -77 -102 686 CA TYR 97 -5.835 ATOM 14.852 65.583 1.000 23.71 ANISOU 686 CA TYR 97 -5.83 ANISOU 686 CA TYR 97 2480 ATOM 687 C TYR 97 -5.02 ANISOU 687 C TYR 97 2363 ATOM 688 O TYR 97 -3.99 ANISOU 688 O TYR 97 2205 3542 2987 -27 106 644 -5.026 15.828 64.743 1.000 23.06 3754 2647 -410 -78 350 -3.992 16.327 65.230 1.000 24.29 TYR 97 2205 3845 3178 -133 -230 7 4 689 CB TYR ATOM 97 -5.585 13.451 65.035 1.000 28.38 ANISOU 689 CB TYR 3230 97 3324 4229 540 -450 8 3 2 690 CG ATOM TYR 97 -4.132 13.025 65.082 1.000 30.37 ANISOU 690 CG TYR 97 3278 97 -3.511 4101 4161 766 -191 6 7 1 ATOM 691 CD1 TYR 12.691 66.285 1.000 30.19 ANISOU 691 CD1 TYR 97 2878 4475 4119 1106 151 951 ATOM 692 CD2 TYR 97 -3.370 12.945 63.922 1.000 29.79 ANISOU 692 CD2 TYR 97 3317 4005 3997 53 - 253 544 ATOM 693 CE1 TYR 97 -2.178 12.294 66.324 1.000 32.77 ANISOU 693 CE1 TYR 97 2554 4771 5126 574 -68 763 MOTA 694 CE2 TYR 97 -2.043 12.553 63.955 1.000 32.68 ANISOU 694 CE2 TYR 97 3536 3793 5087 403 353 323 695 ATOM CZTYR 97 -1.445 12.228 65.157 1.000 33.00 ANISOU 695 CZ TYR 97 2633 4284 5622 1066 264 456 696 OH TYR ATOM 97 -0.121 11.845 65.156 1.000 42.66 ANISOU 696 OH TYR 97 2572 5373 8264 1161 764 1277 ATOM CB SER 697 98 -3.465 16.575 62.134 1.000 23.20 ANISOU 697 CB SER 98 2461 2766 3587 105 698 OG SER ATOM 98 -3.632 15.649 61.078 1.000 26.49 ANISOU 698 OG SER 98 3824 3059 3180 -154 238 -457

-5.694

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17.744 61.701 1.000 18.66

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- 113 -ANISOU 702 CA SER 98 2430 2637 2982 153 294 13.3 703 N MET 99 -5.307 18.891 61.148 1.000 18.68 ANISOU 703 N 99 2392 MET 2722 1984 -978 -366 1 0 1 704 CA MET -6.047 19.560 60.075 1.000 17.84 ATOM 99 ANISOU 704 CA MET 99 2431 2620 1726 -945 -212 - 17 ATOM 705 CB MET -6.819 20.779 60.585 1.000 19.71 99 ANISOU 705 CB MET 99 2348 2968 2173 -679 25 6 4 MET ATOM 706 CG 99 -8.052 20.392 61.374 1.000 23.68 2360 ANISOU 706 CĠ MET 99 3055 3582 -504 393 489 -9.031 21.821 61.911 1.000 22.33 ATOM 707 SD MET 99 MET ANISOU 707 2569 3383 2534 -522 170 -1 -8.148 22.225 63.419 1.000 36.98 SD 99 -522 170 -120 708 MET ATOM CE 99 99 6485 4165 3401 -225 -1904 99 -5.070 19.954 58.973 1.000 17.19 ANISOU 708 CE MET -225 -1904 - 23 709 MOTA С MET 99 2269 MET 99 2269 2488 1776 -960 -194 - 201 MET 99 -3.964 20.341 59.324 1.000 16.93 ANISOU 709 C 710 0 ATOM ANISOU 710 O 710 O MET 99 1932 2583 1919 -367 -208 - 2711 N CYS 100 -5.486 19.864 57.715 1.000 20.00 -3*F*7 -208 - 241 ATOM ANISOU 711 N CYS 100 3178 2683 1739 -1753 -358 1 ATOM 712 CA CYS 100 -4.645 20.181 56.554 1.000 16.64 ANISOU 712 CA CYS 100 2213 2294 1817 -924 -563 4 ATOM 713 CB CYS 100 -4.291 18.893 55.813 1.000 17.74 -1753 -358 1 6 6 1817 -924 -563 4 6 8 100 -4.291 18.893 55.813 1.000 17.74 ANISOU 713 
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 CB CYS 100 2161 -765 1 0 5 3 CYS CYS 714 SG ATOM 100 5244 ANISOU 714 SG 100 5244 3511 3997 414 1509 6 100 -5.347 21.121 55.590 1.000 13.48 1509 6 0 1 CYS MOTA 715 C 100 1879 1415 1829 -68 240 -100 -6.585 21.127 55.496 1.000 14.49 100 1880 1952 1672 ANISOU 715 C CYS 240 - 91ATOM 716 O CYS ANISOU 716 O CYS 100 1880 1952 -497 -57 1 4 1673 N TYR 101 -4.589 21.921 54.852 1.000 13.35 N TYR 101 1721 1677 1673 -254 -78 4 CA TYR 101 -5.016 22.753 53.755 1.000 10.27 ATOM 717 N ANISOU 717 N 1673 -254 -78 4 9 718 ATOM ANISOU 718 CA TYR 101 926 1498 1477 -15 -141 -231 TYR 101 926 1498 1477 -15 -141 -231
TYR 101 -5.102 24.265 54.124 1.000 13.60
TYR 101 1626 1513 2027 -48 322 -23
TYR 101 -5.498 25.025 52.863 1.000 17.31
TYR 101 2373 1509 2694 -158 -103 1 9 3
TYR 101 -6.815 25.068 52.519 1.000 16.38
TYR 101 2464 752 3006 190 -227 5 5
TYR 101 -7.307 25.715 51.412 1.000 17.01 ATOM 719 CB ANISOU 719 СB -48 322 -236 MOTA 720 ČG TYR ANISOU 720 CG ATOM 721 CD1 TYR ANISOU 721 CD1 TYR ATOM 722 CE1 TYR ANISOU 722 CE1 TYR 101 2755 101 2755 714 2993 -86 -416 1 2 2 101 -4.616 25.679 52.012 1.000 19.51 ATOM 723 CD2 TYR CD2 TYR 101 3032 ANISOU 723 1533 2847 -1143 -594 4 7 5 724 CE2 TYR 101 -5.065 26.321 50.872 1.000 20.96 MOTA ANISOU 724 CE2 TYR 101 2802 724 CE2 TYR 101 2802 1949 3211 238 112 769 725 CZ TYR 101 -6.414 26.334 50.568 1.000 22.78 ATOM CZ TYR 101 -6.414 26.334 50.568 1.000 22.78
CZ TYR 101 3238 2291 3126 -1228 -919 6 2
OH TYR 101 -6.875 26.986 49.442 1.000 23.10
OH TYR 101 3141 3112 2522 -14 -129 4 2
C TYR 101 -4.041 22.518 52.596 1.000 11.25
C TYR 101 1223 1398 1654 -323 103 -2
O TYR 101 -2.823 22.677 52.787 1.000 12.23
O TYR 101 1114 1750 1784 -87 130 -2
N SER 102 -4.542 22.190 51.405 1.000 11.17
N SER 102 1355 1279 1611 -220 145 -2 ANISOU 725 3126 -1228 -919 6 2 4 MOTA 726 ANISOU 726 -14 -129 4 2 9 727 ATOM ANISOU 727 -323 103 -252 728 0 ATOM ANISOU 728 O 130 - 20 ATOM 729 N ANISOU 729 N 102 13,55 SER 1279 1611 -220 145 - 263 102 -3.752 21.802 50.235 1.000 10.46 ATOM 730 CA SER ANISOU 730 CA SER 102 1144 1263 1568 62 -1 -125 102 -4.027 20.343 49.908 1.000 13.46 ATOM 731 CB SER ANISOU 731 CB SER 102 1668 1212 2234 324 105 - 301 102 -3.723 19.487 51.025 1.000 16.42 102 2291 1313 2637 -122 -43 9 MOTA 732 OG SER ANISOU 732 OG SER -122 - 43 9 6

- 114 -ATOM 733 C SER 102 -4.046 22.668 49.008 1.000 11.74 ANISOU 733 C SER 102 1346 1500 1614 18 - 39 - 10 734 O SER 102 -5.148 23.148 48.784 1.000 12.84 ATOM ANISOU 734 O SER 102 1480 1410 1988 90 -66 249 ATOM 735 Ν MET 103 -3.004 22.871 48.187 1.000 12.33 ANISOU 735 Ν MET 103 1554 1722 1409 -262 -10 -246 736 ATOM CA MET 103 -3.188 23.603 46.938 1.000 12.92 ANISOU 736 CA MET 103 1663 1681 1565 22 47 - 70 737 ATOM CВ MET 103 -3.215 25.122 47.179 1.000 17.51 ANISOU 737 СВ MET -363 812 - 44 738 CG MET ANISOU 738 CG MET 103 2509 1470 3646 -538 688 376 27.614 47.689 1.000 18.10 ATOM 739 103 -2.136 MET ANISOU 739 MET 103 2235 -3 -334 - 352 ATOM 740 CE MET ANISOU 740 CE MET 103 2319 1457 ATOM 741 C ANISOU 741 C ATOM 742 O ANISOU 742 O ATOM 743 N ANISOU 743 N 3098 -187 -718 -214 103 -2.152 23.221 45.892 1.000 12.57 MET 103 1420 1837 1519 119 -53 2 3 8 103 -1.120 22.573 46.175 1.000 12.57 103 1094 1891 1792 -155 -165 2 7 6 104 -2.418 23.650 44.655 1.000 12.83 104 1493 1958 1422 237 -124 - 3 4 104 -1.533 23.459 43.513 1.000 12.65 104 1075 2188 1544 -93 -37 2 4 2 MET MET MET  ${ t GLY}$ GLYATOM 744 CA GLY ANISOU 744 CA GLY ATOM 745 C GLY 104 1075 2188 1544 -93 -37 2 104 -1.624 24.622 42.542 1.000 14.36 -93 -37 242 ANISOU 745 C GLY104 1909 1985 1561 -265 -294 1 4 2 104 -2.033 25.700 42.967 1.000 15.69 104 1909 ATOM 746 O GLY
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 105 -0.359
 25.083
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 THR ANISOU 749 CB THR -37 -106 5 5 4 750 OG1 THR 105 -0.884 23.876 38.446 1.000 16.16 105 1738 2260 105 1.092 24.882 105 1918 2871 ANISOU 750 OG1 THR 2140 217 ATOM 751 CG2 THR 24.882 39.369 1.000 17.47 ANISOU 751 CG2 THR ANISOU 751 CG2 THR
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- 115 -
   ANISOU 763 OD1 ASP 107 3447
                                                                             2970
               U 763 OD1 ASP 107 3447 2970 2672 698 -753 -772
764 OD2 ASP 107 -7.563 21.311 38.080 1.000 24.88
                                      ASP 107 2496 4004 2954 105 244 -6
ASP 107 -8.285 23.785 42.160 1.000 14.16
  ANISOU 764
                           OD2 ASP 107 2496
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  ATOM
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O ASP 107 -8.507 22.850 42.936 1.000 16.67
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  ATOM
  ANISOU 766
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ATOM 768 CA ASN 108 -7.967 25.314 44.031 1.000 13.68
ANISOU 768 CA ASN 108 1479 1823 1898 153 107 2
ANISOU 769 CB ASN 108 -6.925 26.420 44.272 1.000 15.60
ANISOU 769 CB ASN 108 1593 2026 2309 16 267 - 98
ATOM 770 CG ASN 108 -5.516 25.942 43.963 1.000 15.23
                                                                                                                         107 257
 ATOM //O CG ASN 108 -5.310 23.342 23.342 ATOM 770 CG ASN 108 1505 2141 2142 5 -53 2 ATOM 771 OD1 ASN 108 -5.086 24.932 44.505 1.000 15.40
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ATOM 772 ND2 ASN 108 -4.823 26.678 43.094 1.000 16.96

ANISOU 772 ND2 ASN 108 1593 2198 2652 339 393 222

ATOM 773 C ASN 108 -9.310 25.708 44.642 1.000 14.55

ANISOU 773 C ASN 108 1471 1937 2120 261 191 526

ATOM 774 O ASN 108 -10.222 26.170 43.958 1.000 16.89

ANISOU 774 O ASN 108 1861 2336 2219 716 -109 1 4

ATOM 775 N LEU 109 -9.412 25.512 45.954 1.000 13.42

ANISOU 775 N LEU 109 1458 1648 1994 179 130 9

ATOM 776 CA LEU 109 -10.602 25.796 46.769 1.000 13.53

ANISOU 776 CA LEU 109 1094 2122 1923 -52 -86 -256

ATOM 777 CB LEU 109 -11.187 24.499 47.331 1.000 14.50

ANISOU 777 CB LEU 109 1382 1959 2169 119 455 -468
 ANISOU 777 CB LEU 109 1382 1959 2169 119 455 -4
ATOM 778 CG LEU 109 -11.580 23.383 46.370 1.000 15.21
                                                                                                                          455 - 468
ATOM 778 CG LEU 109 -11.580 23.383 46.370 1.000 15.21 ANISOU 778 CG LEU 109 1593 1785 2403 -235 63 - 342 ATOM 779 CD1 LEU 109 -11.931 22.083 47.089 1.000 18.26 ANISOU 779 CD1 LEU 109 2460 1674 2806 382 -414 - 94 ATOM 780 CD2 LEU 109 -12.780 23.783 45.529 1.000 22.36 ANISOU 780 CD2 LEU 109 -12.780 23.783 45.529 1.000 22.36 ATOM 781 C LEU 109 3055 2391 3052 44 -1155 288 ATOM 781 C LEU 109 -10.203 26.794 47.840 1.000 13.54 ANISOU 781 C LEU 109 1179 1989 1979 76 -116 -259 ANISOU 782 O LEU 109 -9.416 26.428 48.717 1.000 16.15 ANISOU 782 O LEU 109 2196 2210 1730 -52 -366 3 2 ATOM 783 N PHE 110 -10.706 28.025 47.786 1.000 16.11 ANISOU 783 N PHE 110 1369 2042 2709 105 -118 -288 ATOM 784 CA PHE 110 1369 2042 2709 105 -118 -288 ANISOU 784 CA PHE 110 1626 1801 3050 -116 259 -362
ANISOU 783 N PHE
ATOM 784 CA PHE
ANISOU 784 CA PHE
ATOM 785 CB PHE
ANISOU 785 CB PHE
ANISOU 786 CG PHE
ANISOU 786 CG PHE
ATOM 787 CD1 PHE
ANISOU 787 CD1 PHE
ANISOU 788 CD2 PHE
ANISOU 788 CD2 PHE
ANISOU 789 CE1 PHE
ANISOU 789 CE1 PHE
                                              110 1702 2650
                                              110 1702 2650 3368 -176 459 -
110 -7.257 29.598 47.793 1.000 20.35
                                                                                                             -176 459 -385
                                              461 573 - 707
                                                                                                             512 712 - 264
                                               110 1958 2116 3332 176 749 -6
110 -7.288 29.846 45.050 1.000 20.65
110 2158 2094 3596 370
 ANISOU 789 CE1 PHE
                                                                                                             176 749 -631
 ATOM 790 CE2 PHE
 ANISOU 790 CE2 PHE
                                               110 2158 2094 3596 758 724 - 110 -6.118 29.496 45.694 1.000 19.43
                                                                                                                           724 - 321
            791 CZ PHE
ATOM
ANISOU 791 CZ PHE
                                               110 1925
                                               110 1925 2131 3327 219 542 - 110 -11.495 29.556 49.538 1.000 17.08
                                                                                                                           542 - 780
ATOM 792 C
                                    PHE
ANISOU 792 C
                                    PHE 110 1774 1806 2911 -74 414 -111
PHE 110 -12.562 29.792 48.929 1.000 21.26
ATOM 793 O
ANISOU 793 O
                                    PHE 110 1849
                                                                           2577
                                                                                            3650 405 178 -448
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- 116 -

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794 N
                 PRO 111 -11.406 29.717 50.851 1.000 19.41
PRO 111 2279 2110 2985 -386 519 -
 ANISOU 794 N
                                                -386 519 -314
        795 CD PRO 111 -10.278 29.322 51.705 1.000 19.20
 ANISOU 795 CD PRO
                     111 2773
                                 1880
                                         2640
                                               -417 255 -514
        796 CA
 ATOM
                     111 -12.549 30.252 51.604 1.000 21.47
                PRO
 ANISOU 796 CA
                PRO
                     111 3025
                                 1924
                                         3206 -50
                                                     728 -635
                     111 -12.167 30.007 53.055 1.000 23.63
        797
 ATOM
            СВ
                PRO
 ANISOU 797
            CB
                PRO
                     111 3789
                                 2054
                                         3137
                                                334 776 - 575
            СG
                     111 -10.775 29.535 53.100 1.000 22.33
 ATOM
        798
                PRO
 ANISOU 798
            CG
                PRO
                     111 2767
                                 2908
                                        2809
                                                -1006 623 -414
                     111 -12.828 31.739 51.433 1.000 23.88
 ATOM
        799
            С
                 PRO
 ANISOU 799
            C
                 PRO
                     111 3139
                                 2049
                                        3887
                                                79 -142 -479
        800
            0
 MOTA
                     111 -13.919 32.194 51.834 1.000 26.77
                 PRO
 ANISOU 800 O
                PRO
                     111 3800
                                 2818
                                        3555
                                                992 -91 -397
 ATOM
        801
           N
                     112 -11.906 32.517 50.872 1.000 25.19
                SER
 ANISOU 801
           N
                SER
                     112 3514
                                 2269
                                        3788
                                                -247 -856 282
 ATOM
       802
                     112 - 12.300 33.919 50.631 1.000 26.43
            CA
                SER
 ANISOU 802
            CA
                SER
                     112 2654
                                 2655
                                        4734
                                               496
       803
                     112 -12.506 34.712 51.912 1.000 33.37
 ATOM
            СВ
                SER
 ANISOU 803
            CВ
                SER
                     112 3122
                                 3663
                                        5895
                                               172
                                                     2582 ~ 510
                     112 -11.322 34.719 52.688 1.000 36.94
 MOTA
       804
            OG
                SER
 ANISOU 804
            OG
                SER
                     112 6530
                                 2154
                                        5351
                                               1399
                                                     206 - 415
       805
            C
ATOM
                SER
                     112 -11.262 34.587 49.723 1.000 26.62
ANISOU 805
                SER
                     112 2613
                                 2546
                                        4956
                                               1021
                                                     1668 6 5 1
            0
ATOM
       806
                     112 -10.219 34.029 49.414 1.000 22.81
                SER
ANISOU 806
            0
                SER
                     112 2241
                                 2782 3645
                                               800
                                                     837 - 400
       807 N
ATOM
                \operatorname{GLY}
                     113 -11.570 35.802 49.279 1.000 28.93
ANISOU 807 N
                     113 2937 2947 5108 1008 1175 1
113 -10.659 36.478 48.365 1.000 30.79
                \operatorname{GL} Y
                                               1008 1175 1198
       808 CA GLY
ATOM
ANISOU 808 CA GLY
                     113 2992
                                 3606 5102 381 798 1
36.829 49.070 1.000 31.83
                                                     798 1400
       809 C
ATOM
                     113 -9.362
                GLY
ANISOU 809 C
                GLY
                     113 3297
                                 3919
                                        4878
                                               262 897 528
ATOM
       810 O GLY
                                 36.790 48.459 1.000 25.85
                     113 -8.294
ANISOU 810 O GLY
                     113 2920
                                 2317
                                        4585
                                               857 450 - 203
       811
MOTA
            N
                ASP
                     114 -9.479
                                 37.145 50.365 1.000 29.56
ANISOU 811
            N
                ASP
                     114 3487
                                 2877
                                        4868
                                               866
                                                     1104 7 6 0
            CA ASP
                     114 -8.257
MOTA
       812
                                 37.463 51.122 1.000 26.15
ANISOU 812
                     114 3189
                                 2680
                                        4066
                                               1028 1584 5 4 2
ATOM
       813
            CB ASP
                     114 -8.628
                                 37.937 52.526 1.000 33.81
ANISOU 813
            CB
               ASP
                     114 5580
                                 2697
                                        4569
                                               1774 1691 - 240
ATOM
       814
               ASP
            CG
                     114 -7.904
                                 39.232 52.840 1.000 40.77
ANISOU 814
            CG ASP
                     114 6798
                                 3734
                                        4960
                                               719
                                                     693 - 248
ATOM
       815
            OD1 ASP
                     114 -8.330
                                 40.277
                                        52.295 1.000 48.61
ANISOU 815 OD1 ASP
                     114 6014
                                        9920
                                 2534
                                               1703 931 -913
       816 OD2 ASP
ATOM
                     114 -6.932
                                 39.178 53.622 1.000 54.35
ANISOU 816
            OD2 ASP
                     114 5258
                                 7609
                                        7783
                                               -868 495 1602
       817
MOTA
            С
                ASP
                     114 -7.310 36.281 51.231 1.000 23.05
ANISOU 817
            С
                ASP
                     114 2621
                                 2102
                                        4033
                                               444
                                                     1874 3 4 0
       818
ATOM
            0
                ASP
                     114 -6.111
                                 36.371 50.955 1.000 22.05
ANISOU 818
            0
                ASP
                     114 2423
                                 2277
                                        3677
                                               131
                                                     1411 - 461
ATOM
       819
            N
                PHE
                     115 -7.854
                                 35.160 51.637 1.000 23.21
ANISOU 819
            N
                PHE
                     115 2945
                                 1890
                                        3984
                                               -130 1293 - 228
- ATOM
       820
            CA PHE
                     115 -7.120
                                 33.896 51.690 1.000 19.93
ANISOU 820
            CA PHE
                     115 2562
                                 1908
                                        3102
                                               -198 655 -294
MOTA
       821
            CВ
               PHE
                     115 -8.085
                                 32.792 52.157 1.000 19.49
ANISOU 821
            CB
               PHE
                     115 2378
                                 1754
                                        3275
                                               64 881 - 314
MOTA
       822
            CG
                PHE
                     115 -7.523
                                 31.445 52.540 1.000 17.25
ANISOU 822
            CG
               PHE
                     115 2053
                                 1589
                                        2912
                                               -56 348 -695
ATOM
       823
            CD1 PHE
                     115 -7.637
                                 30.951 53.833 1.000 19.00
ANISOU 823
            CD1 PHE
                     115 2728
                                 1539
                                        2950
                                               73 496 - 683
MOTA
       824
            CD2 PHE
                     115 -6.868 30.634 51.615 1.000 17.88
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- 117 -ANISOU 824 CD2 PHE 115 1933 1931 2927 7 298 -810 ATOM 825 CE1 PHE 115 -7.100 29.711 54.163 1.000 20.25 ANISOU 825 CE1 PHE 115 2825 1825 3042 317 341 -575 ATOM 826 CE2 PHE 115 -6.338 29.412 51.955 1.000 19.11 ANISOU 826 CE2 PHE 115 1865 2158 3237 336 351 -885

- 118 -855 CD1 ILE 118 -3.786 37.025 53.582 1.000 29.63 CD1 ILE 118 6169 3096 1994 189 1258 -ANISOU 855 CD1 ILE 3096 1994 189 1258 - 1068 118 -1.692 34.172 49.959 1.000 15.65 856 C ILE 118 2316 ANISOU 856 C ILE -89 573 -117 ATOM 857 O ILE ANISOU 857 O 118 2240 ILE 1255 2051 16 286 2 1 4 119 -2.523 33.139 49.784 1.000 14.44 ATOM 858 N TRP ANISOU 858 N TRP 119 2125 1592 1771 47 128 - 7 1 119 -2.010 31.795 49.518 1.000 13.68 ATOM 859 CA TRP ANISOU 859 CA TRP 119 1712 1529 1957 -61 220 4 0 119 -3.089 30.755 49.932 1.000 14.93 860 CЗ TRP ANISOU 860 CB TRP 119 1819 1729 2123 -234 295 - 35 119 -2.864 30.482 51.420 1.000 16.19 119 1819 ATOM 861 CGTRP ANISOU 861 CG TRP 119 1640 2364 2146 -168 582 167 119 -2.116 29.430 51.993 1.000 20.41 ATOM CD2 TRP 862 ANISOU 862 CD2 TRP 119 3189 2414 2151 202 523 405 863 CE2 TRP 119 -2.177 29.580 53.392 1.000 19.84 ANISOU 863 CE2 TRP 119 3536 1818 2184 -439 234 137 ATOM 864 CE3 TRP 119 -1.390 28.357 51.456 1.000 23.94 ANISOU 864 CE3 TRP 119 5382 1647 2068 561 126 400 ATOM 865 CD1 TRP 119 -3.340 31.223 52.460 1.000 20.05 ANISOU 865 CD1 TRP 119 3207 2343 2069 -9 189 -139 ATOM 866 NE1 TRP 119 -2.938 30.689 53.649 1.000 20.32 ANISOU 866 NE1 TRP 119 2806 2726 2188 -96 -68 -185 ATOM 867 CZ2 TRP 119 -1.547 28.714 54.281 1.000 22.12 ANISOU 867 CZ2 TRP 119 4071 2256 2078 -17 105 2 2 ATOM 868 CZ3 TRP 119 -0.761 27.490 52.332 1.000 21.52 ANISOU 868 CZ3 TRP 119 4214 119 -0.847 2168 1794 - 311-193 1 9 7 CH2 TRP ATOM 869 27.674 53.715 1.000 24.34 ANISOU 869 CH2 TRP 2047 1850 329 148 183 31.634 48.095 1.000 14.27 1259 1985 7 -187 334 -65 119 5349 ATOM 870 C TRP 119 -1.521 ANISOU 870 C ATOM 871 O TRP 119 2180 119 -0.569 30.865 47.855 1.000 14.73 TRP ATOM 871 O ANISOU 871 O ATOM 872 N ANISOU 872 N ATOM 873 CA ANISOU 873 CA ATOM 874 CB TRP 119 1996 119 1996 1653 1946 -67 362 1 120 -2.109 32.325 47.116 1.000 13.99 1653 -67 362 101 THR THR 120 2231 1237 1848 106 627 - 137 THR 120 -1.541 32.275 45.762 1.000 15.19 THR 120 1903 2093 1774 9 435 - 242 THR 120 -2.492 32.983 44.787 1.000 16.41 ANISOU 874 CB THR 120 1934 2304 1995 -331 152 6 6 875 OG1 THR ATOM 120 -3.738 32.297 44.766 1.000 18.53 ANISOU 875 OG1 THR 2288 2863 -236 195 4 32.906 43.358 1.000 18.02 120 1891 -236 195 407 ATOM 876 CG2 THR 120 -1.974 ANISOU 876 CG2 THR ATOM 877 C ANISOU 877 C ATOM 878 O ANISOU 878 O ATOM 879 N 120 2135 2602 2108 324 322 318 120 -0.145 32.870 45.727 1.000 14.19 THR THR 120 1868 2050 1475 87 285 - 167 THR 120 0.756 32.299 45.078 1.000 13.62 THR 120 1864 1692 1620 301 354 217 GLN 121 0.114 33.962 46.429 1.000 14.55 ANISOU 879 N 121 1721 GLN 1672 2136 304 175 - 67 880 CA GLN ATOM 121 1.459 ANISOU 880 CA GLN 34.548 46.483 1.000 15.80 121 2.465 121 2.465 121 1747 121 3.603 121 2063 1666 2271 -18 -119 3 6 2 ATOM 881 C GLN 33.642 47.176 1.000 13.73 ANISOU 881 C GLN 1665 1806 -30 ATOM 882 Q GLN 33.452 46.685 1.000 15.36 ANISOU 882 O GLN ATOM 883 CB GLN 2084 1688 48 360 - 44 121 1.315 35.918 47.154 1.000 18.85 ANISOU 883 CB GLN 121 2537 1426 3200 -73 -5 3 5 6 ATOM 884 121 2.639 ÇG GLN36.558 47.543 1.000 18.88 ANISOU 884 CG GLN121 2507 1788 2878 599 - 248 ATOM 885 CDGLN 36.936 46.337 1.000 20.70 121 3.468

- 119 -ANISOU 885 CD GLN 121 2584 2138 3142 -373 -85 231 886 OE1 GLN 121 2.935 37.088 45.224 1.000 22.47 OE1 GLN 121 2695 2822 3019 -245 0 121 NE2 GLN 121 4.779 37.101 46.522 1.000 25.22 NE2 GLN 121 2426 3344 3811 127 -131 13 N TYR 122 2.081 33.054 48.299 1.000 12.26 N TYR 122 1747 1514 1399 99 -55 - 258 ANISOU 886 -245 0 121 MOTA 887 ANISOU 887 127 -131 1385 888 N ATOM ANISOU 888 N 1514 1399 99 -55 - 258 32.102 49.050 1.000 13.18 889 CA TYR 122 2.896 32.10 1643 1724 ATOM ANISOU 889 CA TYR 122 1901 1464 -20 -253 - 160 31./2 1435 2 808 890 CB TYR 122 2.211 ATOM 31.724 50.364 1.000 13.78 ANISOU 890 CB TYR 122 2045 1756 116 48 - 28 891 CG TYR 122 2.994 30.808 51.282 1.000 14.22 891 CG TYR 122 1966 1681 1758 101 68 1 0 ATOM ANISOU 891 CG TYR 122 1966 1681 1758 101 68 101 ATOM 892 CD1 TYR 122 4.271 31.120 51.722 1.000 17.48 ANISOU 892 CD1 TYR 122 1788 1972 2882 149 -5 4 20 ATOM 893 CE1 TYR 122 5.003 30.284 52.576 1.000 18.55 ANISOU 893 CE1 TYR 122 2131 2050 2868 102 -404 2 5 1 ATOM 894 CD2 TYR 122 2.445 29.619 51.731 1.000 20.72 ANISOU 894 CD2 TYR 122 3308 1366 3197 -519 -1524 3 2 3 ATOM 895 CE2 TYR 122 3.140 28.773 52.574 1.000 25.40 ANISOU 895 CE2 TYR 122 3.772 1812 4067 -782 -2084 8 7 3 ANISOU 896 CZ TYR 122 4.413 29.101 52.992 1.000 20.93 ANISOU 896 CZ TYR 122 2985 1742 3224 -96 -1145 3 1 3 ATOM 897 OH TYR 122 5.068 28.230 53.826 1.000 29.87 ANISOU 897 OH TYR 122 4830 1998 4522 -680 -3078 6 2 1 ATOM 898 C TYR 122 3.218 30.876 48.209 1.000 12.33 ANISOU 898 C TYR 122 1833 1412 1439 89 -218 8 8 ANISOU 891 898 C TYR 122 3.218 30.876 48.209 1.000 12.33
898 C TYR 122 1833 1412 1439 89-218 8 8
899 O TYR 122 4.395 30.507 48.117 1.000 14.25
899 O TYR 122 1896 1861 1656 339 -242 2 1 6
900 N PHE 123 2.224 30.269 47.573 1.000 11.28
900 N PHE 123 1950 1297 1041 6 -151 1 8 5
901 CA PHE 123 2.482 29.151 46.665 1.000 12.08
901 CA PHE 123 1731 1219 1640 64 -60 2 6
902 CB PHE 123 1.139 28.719 46.024 1.000 13.86
902 CB PHE 123 2048 1550 1666 -104 -276 - 8 2
903 CG PHE 123 1.311 27.516 45.099 1.000 14.44
903 CG PHE 123 1.281 27.516 45.099 1.000 14.44
904 CD1 PHE 123 1.281 26.234 45.614 1.000 13.64
904 CD1 PHE 123 1857 1563 1764 -42 -702 - 23 6
905 CD2 PHE 123 1.511 27.664 43.729 1.000 13.81 ANISOU 898 C ATOM 899 O ANISOU 899 O ATOM 900 N ANISOU 900 N MOTA ANISOU 901 CA PHE ANISOU 902 ATOM ANISOU 903 ATOM ANISOU 904 CD1 PHE ATOM ANISOU 905 ATOM ANISOU 906 ATOM ANISOU 907 CE2 PHE ANISOU 908 CZ PHE ATOM 909 C PHE ANISOU 909 C ATOM ANISOU 910 O PHE 123 1591 ATOM ANISOU 911 N MOTA ANISOU 912 ASP 124 3.708 32.352 43.242 1.000 18.95 ASP 124 2650 1970 2580 656 -63 92 ASP 124 4.470 32.708 41.989 1.000 27.54 ATOM 124 3.705 124 2650 124 4.470 124 4.470 124 5327 124 4.541 124 6362 125 80 126 656 127 2099 128 939 129 3036 120 37 04 124 6362 125 4485 108 2616 - 3 ANISOU 913 СB 656 -63 9 2 6 ATOM 914 CG ANISOU 914 ASP CG -123 939 880 915 OD1 ASP ATOM ANISOU 915 OD1 ASP 108 2616 - 331

- 120 -916 OD2 ASP ATOM 124 4.985 33.843 42.011 1.000 32.60 ANISOU 916 OD2 ASP 124 4724 3509 4151 -1539 234 851 ATOM 917 С 124 5.645 ASP 31.164 44.328 1.000 14.49 917 C 918 O 918 O 919 N ANISOU 917 ASP 124 1493 1721 2293 327 485 482 ATOM ASP 124 6.591 30.721 43.674 1.000 14.52 ANISOU 918 ASP 124 1477 1363 2679 289 497 307 ATOM ARG 125 5.866 31.777 45.499 1.000 14.03 ANISOU 919 N ARG 125 1501 1271 2558 353 398 414 ATOM 920 31.863 46.044 1.000 16.40 CAARG 125 7.214 ANISOU 920 CAARG 125 1642 1625 2963 194 178 226 921 ATOM C 30.494 46.346 1.000 14.69 125 7.828 125 1396 ARG ANISOU 921 С ARG 1688 2496 232 -25 153 MOTA 922 0 125 8.999 ARG 30.245 46.034 1.000 14.10 ANISOU 922 O. ARG 125 1279 1656 2424 7 -205 -201 ATOM 923 CB 125 7.213 ARG 32.705 47.318 1.000 18.13 ANISOU 923 125 1950 CB ARG 1902 3035 -81 4 6 787 ATOM 924 CG ARG 125 7.045 34.193 47.041 1.000 23.51 ANISOU 924 CG ARG 125 2232 1780 4919 883 -36 - 225ATOM 925 CD ARG 125 8.391 34.815 46.694 1.000 29.33 ANISOU 925 CD ARG 125 3596 2824 4724 -667 237 -187 ATOM 926 ΝE ARG 125 8.194 36.262 46.803 1.000 32.99 ANISOU 926 NE ARG 125 4350 2766 5418 -678 -1642 156 ATOM 927 CZARG 125 8.868 37.153 47.495 1.000 27.38 CZ ARG ANISOU 927 125 2292 2758 5353 -276 -580 - 246 ATOM 928 NH1 ARG 125 9.916 36.821 48.235 1.000 38.55 ANISOU 928 NH1 ARG 125 4611 3604 6433 449 -2476 -669 ATOM 929 NH2 ARG 125 8.491 38.423 47.442 1.000 30.26 ANISOU 929 NH2 ARG 125 4062 4865 2570 -369 -835 3 6 3 930 ATOM 126 7.065 М  ${ t GLN}$ 29.573 46.920 1.000 12.36 ANISOU 930 N GLN 126 1316 1376 2002 248 -63 -264 ATOM 931 CA GLN 126 7.524 28.201 47.153 1.000 13.39 ANISOU 931 CA GLN 126 1765
CB AGLN 126 6.363
CB AGLN 126 6.363 1323 1999 219 -355 - 377 ATOM 932 27.455 47.828 0.500 16.24 ANISOU 932 CВ AGLN 126 2422 -1391 2357 188 202 - 192 ATOM 933 AGLN 126 6.149 CG 27.758 49.284 0.500 18.83 ANISOU 933 AGLN 126 2761 CG 2021 2371 68 233 - 210 ATOM 934 AGLN 126 7.077 CD27.146 50.298 0.500 23.94 ANISOU 934 CD AGLN 126 3578 2745 2774 -604 -757 3 3 ATOM 935 OE1 AGLN 126 7.181 27.683 51.419 0.500 35.94 ANISOU 935 OE1 AGLN 126 6788 3731 3136 -578 -1567 -478 936 MOTA NE2 AGLN 126 7.774 26.055 50.008 0.500 24.63 ANISOU 936 NE2 AGLN 126 4491 1118 3751 -881 -2407 462 ATOM 937 CB BGLN 126 6.525 27.417 48.018 0.500 13.36 ANISOU 937 CB BGLN 126 1695 1137 2245 602 -114 - 255 ATOM 938 CG BGLN 126 6.604 27.750 49.497 0.500 18.28 ANISOU 938 CG BGLN 126 2537 2257 2153 -68 -176 - 105 ATOM 939 CD BGLN 126 5.442 27.237 50.319 0.500 18.42 CD BGLN 126 2227 ANISOU 939 2573 2198 344 OE1 BGLN 126 5.605 OE1 BGLN 126 3289 -159 1 0 6 ATOM 940 26.442 51.242 0.500 25.36 ANISOU 940 3517 2828 -100 -223 9 5 3 ATOM NE2 BGLN 126 4.231 941 27.685 50.003 0.500 25.02 ANISOU 941 NE2 BGLN 126 2427 2669 4413 1004 -83 -298 942 ATOM C 126 7.860 GLN 27.448 45.861 1.000 12.95 ANISOU 942 C GLN 126 1506 1434 1979 307 -372 - 366 ATOM 943 O. 126 8.859 GLN 26.721 45.748 1.000 11.66 ANISOU 943 0 GLN 126 1461 1142 1827 182 -85 159 ATOM 944 N TYR 127 6.960 27.578 44.868 1.000 11.61 ANISOU 944 Ν TYR 127 1400 1276 1735 146 -168 - 10 ATOM 945 CATYR 127 7.152 26.869 43.585 1.000 11.21 ANISOU 945 CATYR 127 1469 1242 1550 -92 -40 192 MOTA 946 CB TYR 127 5.901 26.940 42.724 1.000 11.82

- 121 -

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ANISOU 946 CB. TYR 127 1346
                                                                                                                                                                   1655
                                                                                                                                                                                                            1491
                                                                                                                                                                                                                                              -13
                                                                                                                                                                                                                                                                        82 4 7
                                   947
       ATOM
                                                               CG TYR 127 5.791 26.069 41.496 1.000 11.49
       ANISOU 947
                                                               CG TYR 127 1278
                                                                                                                                                                 1428 1660
                                                                                                                                                                                                                                               -4 - 4 1 0
                                                               CD1 TYR 127 6.550 24.928 41.270 1.000 11.28
       ATOM
                                   948
     ANISOU 948 CD1 TYR 127 1030 1334 1921 -87 -100 3 3 ATOM 949 CE1 TYR 127 6.406 24.153 40.115 1.000 11.47 ANISOU 949 CE1 TYR 127 1164 1167 2027 -51 -53 2 1 ATOM 950 CD2 TYR 127 4.871 26.410 40.500 1.000 11.98 ANISOU 950 CD2 TYR 127 4.715 25.655 39.357 1.000 11.37 ANISOU 951 CE2 TYR 127 4.715 25.655 39.357 1.000 11.37 ANISOU 951 CE2 TYR 127 1539 1118 1665 140 -68 - 73 ATOM 952 CZ TYR 127 5.494 24.508 39.163 1.000 11.02 ANISOU 952 CZ TYR 127 1202 1226 1760 91 48 -125 ATOM 953 OH TYR 127 5.379 23.720 38.030 1.000 11.57 ANISOU 953 OH TYR 127 5.379 23.720 38.030 1.000 11.57 ANISOU 953 OH TYR 127 1547 1138 1712 94 177 - 3 ANISOU 954 C TYR 127 8.386 27.392 42.882 1.000 10.83 ANISOU 954 C TYR 127 1296 989 1830 230 -43 3 7 8
       ANISOU 948
                                                               CD1 TYR 127 1030 1334 1921 -87 -100 3 3
                                                                                                                                                                                                                                             204 -219 - 100
   ATOM 954 C TYR 127 8.386 27.392 42.882 1.000 10.83

ANISOU 954 C TYR 127 1296 989 1830 230 -43 3 7 8

ATOM 955 O TYR 127 9.185 26.605 42.375 1.000 10.86

ANISOU 955 O TYR 127 1292 1232 1603 164 -237 - 4 2

ATOM 956 N THR 128 8.565 28.716 42.865 1.000 10.98

ANISOU 956 N THR 128 1554 976 1642 212 -9 5 5 7

ATOM 957 CA THR 128 9.766 29.305 42.295 1.000 11.80

ANISOU 957 CA THR 128 1686 1125 1673 -47 -169 3 8 6

ANISOU 958 CB THR 128 9.605 30.849 42.378 1.000 12.66

ANISOU 958 CB THR 128 1873 1074 1864 -52 -233 5 2 1

ATOM 959 OG1 THR 128 8.530 31.286 41.517 1.000 16.74

ANISOU 959 OG1 THR 128 2223 1597 2542 124 -457 9 9 8

ATOM 960 CG2 THR 128 10.878 31.510 41.893 1.000 16.54
    ANISOU 959 OG1 THR 128 2223 1597 2542 124 -457 9 9 8 ATOM 960 CG2 THR 128 10.878 31.510 41.893 1.000 16.54 ANISOU 960 CG2 THR 128 1871 778 3635 262 655 1 3 8
  ANISOU 960 CG2 THR 128 1871 778 3635 262 655 136 ATOM 961 C THR 128 11.040 28.828 42.964 1.000 11.26 ANISOU 961 C THR 128 1562 980 1738 -71 -162 148 ATOM 962 O THR 128 11.995 28.458 42.258 1.000 12.16 ANISOU 962 O THR 128 1769 1092 1758 17 26 27 9 ATOM 963 N ALA 129 11.083 28.802 44.300 1.000 10.39 ANISOU 963 N ALA 129 11.083 1001 1763 70 -118 147 ATOM 964 CA ALA 129 12.273 28.386 45.037 1.000 10.59 ANISOU 964 CA ALA 129 12.273 28.386 45.037 1.000 10.59 ANISOU 965 CB ALA 129 12.113 28.603 46.536 1.000 12.46 ANISOU 965 CB ALA 129 12.113 28.603 46.536 1.000 12.46 ANISOU 965 CB ALA 129 12.575 26.906 44.802 1.000 11.35 ANISOU 966 C ALA 129 12.575 26.906 44.802 1.000 11.35 ANISOU 966 C ALA 129 1258 883 2170 -16 -141 410 ATOM 967 O ALA 129 13.738 26.485 44.641 1.000 10.93
ANISOU 966 C ALA 129 12.575 26.906 44.802 1.000 11.35
ATOM 967 O ALA 129 13.738 26.485 44.641 1.000 10.93
ANISOU 967 O ALA 129 1202 1157 1796 -36 -213 1 2 1
ATOM 968 N SER 130 11.519 26.086 44.750 1.000 12.27
ANISOU 968 N SER 130 1280 984 2398 -65 -1 - 24
ATOM 969 CA SER 130 11.682 24.650 44.512 1.000 10.89
ANISOU 969 CA SER 130 1623 876 1638 -85 44 3 7 0
ANISOU 970 CB ASER 130 10.342 23.940 44.716 0.500 10.08
ATOM 971 OG ASER 130 1432 603 1793 213 247 4 1 3
ATOM 971 OG ASER 130 1021 651 1792 91 1 - 1 4 3
ATOM 972 CB BSER 130 1021 651 1792 91 1 - 1 4 3
ATOM 973 OG BSER 130 1687 822 1521 -45 318 1 5 8
ATOM 973 OG BSER 130 9.418 24.098 43.734 0.500 16.22
ANISOU 973 OG BSER 130 1717 1289 3156 137 -525 3 4 8
ANISOU 974 C SER 130 12.214 24.373 43 110 1 660
    ANISOU 974 C SER 130 1586 733 1684 -166 210 48 4
ATOM 975 O SER 130 13.137 23.532 42.942 1.000 11.17
ANISOU 975 O SER 130 1385 1012 1849 -151 -95 1 4 0
ATOM 976 N ARG 131 11.680 25.044 42.079 1.000 10.46
    ANISOU 974 C
    ANISOU 975 O SER 130 1385
ATOM 976 N ARG 131 11.680
ANISOU 976 N ARG 131 1578
                                                                                                                                                        861 1534 -87 -66 9 9
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- 122 -CA ARG 131 12.260 24.839 40.742 1.000 10.60 CA ARG 131 1480 1110 1438 61 -288 8 2 CB ARG 131 11.426 25.553 39.679 1.000 12.99 CB ARG 131 1893 1369 1673 63 -525 276 ATOM 977 ANISOU 977 CB ARG 978 ARG 131 1893 1369 1673 63 -525 2 7 6 ARG 131 10.003 25.065 39.431 1.000 13.64 ANISOU 978 63 -525 276 MOTA 979 CG ANISOU 979 CG 131 1707 1735 1742 335 -559 -25.669 38.206 1.000 17.71 ARG 335 -559 - 86 980 CD ATOM ARG 131 9.349 ANISOU 980 CD ARG 131 2078 2677 81 -983 701 1973 27.113 38.015 1.000 19.76 ATOM 981 ΝE ARG 131 9.453 ANISOU 981 ΝE ARG 131 2716 2034 2757 -25 -525 7 1 3 131 8.629 28.004 38.568 1.000 21.24 982 CZARG ANISOU 982 ARG CZ131 3688 1878 2503 -8 -128 647 MOTA 983 NH1 ARG 131 7.631 27.634 39.366 1.000 21.32 ANISOU 983 NH1 ARG 131 2792 3142 2166 -486 -667 5 7 984 131 8.771 29.310 38.361 1.000 27.83 ATOM NH2 ARG ANISOU 984 NH2 ARG 131 4649 1822 4103 -90 -422 5 6 1 985 C 131 13.714 25.323 40.688 1.000 10.42 ARG ANISOU 985 C ARG 131 1542 1078 1339 50 -103 1 24.683 40.080 1.000 10.94 ATOM 986 O ARG 131 14.568 ANISOU 986 O ARG 131 1544 N ALA 132 14.028 26.438 41.343 1.000 10.97 1105 1506 -134 4 2 ATOM 987 ANISOU 987 N ALA 132 1477 1129 74 - 364 - 45 1563 CA ALA 132 15.379 26.983 41.343 1.000 11.10 CA ALA 132 1539 944 1735 9 -102 9 7 ATOM 988 ANISOU 988 ATOM 989 CB ALA 132 15.429 28.344 42.048 1.000 12.82 ANISOU 989 CB ALA 132 1711 1171 1987 -48 -248-1 ATOM 990 C ALA 132 16.393 26.045 41.995 1.000 11.55 ANISOU 990 C ALA 132 1085 1107 2197 -197 305 74 ANISOU 991 O ALA 132 17.481 25.832 41.432 1.000 11.81 ANISOU 991 O ALA 132 1081 1809 1599 -204 17 - 9 -48 -248 -198 1107 2197 -197 305 745 132 1081 1809 1599 -204 17 - 9 133 16.061 25.490 43.175 1.000 11.16 ATOM 992 N ANISOU 992 N VAL 133 1260 133 1260 1356 1623 -148 51 3 5 0 133 17.011 24.587 43.840 1.000 11.62 VAL -148 51 3 5 0 ATOM 993 CA VAL ANISOU 993 CA VAL ATOM 994 CB VAL ANISOU 994 CB VAL 133 1505 1529 1380 -69 -297 8 9 133 16.738 24.418 45.344 1.000 12.14 133 1376 1674 1564 -74 -25 364 995 CG1 VAL 133 15.550 23.501 45.608 1.000 14.96 ATOM ANISOU 995 CG1 VAL 133 1705 2316 1662 -706 8 -357 ATOM 996 CG2 VAL 133 17.981 23.864 46.033 1.000 15.63 ANISOU 996 CG2 VAL 133 1755 2340 1845 -341 -677 5 5 1 ATOM 997 C VAL 133 17.079 23.268 43.065 1.000 11.71 ANISOU 997 C VAL 133 1376 1363 1711 -24 -425 1 6 9 ATOM 998 O VAL 133 18.198 22.733 42.925 1.000 11.55 ANISOU 998 O VAL 133 1391 ATOM 999 N ALA 134 15.982 22.758 42.480 1.000 12.87 ANISOU 999 N ALA 134 1399 1517 1973 28 -334 -22 ATOM 1000 CA ALA 134 16.084 21.557 41.621 1.000 10.57 1453 1545 -4 -116 398 28 -334 -228 ALA 134 1106 1691 153 -298 9 6 MOTA 1001 CB 134 14.699 21.096 41.186 1.000 12.20 ALA ANISOU 1001 CB ALA134 1254 1589 35 - 303 - 127 1794 ATOM 1002 C 134 16.968 21.797 40.399 1.000 12.58 ALA ANISOU 1002 C ALA 134 1393 1399 1987 272 -4 2 7 7 MOTA 1003 0 134 17.712 20.924 39.970 1.000 11.01 ALA ANISOU 1003 O ALA134 1254 1358 1574 83 -268 135 16.908 22.995 39.809 1.000 12.03 MOTA 1004 N ARG ANISOU 1004 N 135 1517 ARG 1230 1824 -62 -327 8 7 1005 CA ARG 135 17.773 23.353 38.676 1.000 13.23 ANISOU 1005 CA 135 1854 ARG 1158 2015 -270 -209 1 6 1 ATOM 1006 CB 135 17.393 24.734 38.170 1.000 14.57 ARG ANISOU 1006 CB ARG 135 2203 1339 1994 -45 -541 2 2 2 MOTA 1007 CG ARG 135 17.753 25.160 36.797 1.000 19.22

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ANISOU 1007 CG ARG 135 4204 1980 1120 -490 -433150ATOM 1008 CD ARG 135 17.237 26.563 36.471 1.000 22.14 ANISOU 1008 CD ARG 135 4046 1500 2868 -159 315 8 ANISOU 1008 CD ARG 135 4046 1500 2868 -159 315 8 ATOM 1009 NE ARG 135 15.831 26.607 36.077 1.000 22.66 ANISOU 1009 NE ARG 135 4239 1404 2965 -94 47 25 -159 315 822 ANISOU 1010 CZ ARG 135 14802 27.184 36.684 1.000 21.69 ANISOU 1010 CZ ARG 135 4004 1906 2333 92 -506 6.4 ATOM 1011 NH1 ARG 135 14.917 27.843 37.833 1.000 22.26 ANISOU 1011 NH1 ARG 135 14.917 27.843 37.833 1.000 22.26 ANISOU 1012 NH2 ARG 135 13.582 27.113 36.149 1.000 22.31 ANISOU 1012 NH2 ARG 135 13.582 27.113 36.149 1.000 22.31 ANISOU 1013 C ARG 135 19.251 23.275 39.057 1.000 12.70 ANISOU 1013 C ARG 135 19.251 23.275 39.057 1.000 12.70 ANISOU 1014 O ARG 135 20.069 22.818 38.238 1.000 14.67 ANISOU 1015 N GLU 136 19.572 23.712 40.266 1.000 12.15 ANISOU 1015 N GLU 136 19.572 23.712 40.266 1.000 12.15 ANISOU 1016 CA GLU 136 16.22 1701 2194 -90 -1973 7 1 ANISOU 1017 CB GLU 136 21.212 24.513 41.981 1.000 22.818 ANISOU 1018 CG GLU 136 21.212 24.513 41.981 1.000 15.59 ANISOU 1018 CG GLU 136 21.012 24.513 41.981 1.000 15.59 ANISOU 1019 CD GLU 136 20.790 27.351 20.700 1.000 12.01 ANISOU 1019 CD GLU 136 20.790 27.351 20.700 20.18 ANISOU 1020 OE1 GLU 136 20.791 20.79 3.519 -308 89 36 9 ANISOU 1020 OE1 GLU 136 20.791 20.79 3.519 -308 89 36 9 ANISOU 1021 OE2 GLU 136 20.71 20.79 3.519 -308 89 36 9 ANISOU 1021 OE2 GLU 136 20.75 20.751 39.670 1.000 14.00 2.4.64 ANISOU 1020 OE1 GLU 136 20.75 20.751 39.670 1.000 14.00 2.4.64 ANISOU 1020 OE1 GLU 136 20.75 20.751 39.670 1.000 14.00 2.4.64 ANISOU 1020 OE1 GLU 136 20.75 20.751 39.670 1.000 24.64 ANISOU 1020 OE1 GLU 136 20.75 20.751 39.670 1.000 24.64 ANISOU 1020 OE1 GLU 136 20.75 20.751 39.670 1.000 24.64 ANISOU 1020 OE1 GLU 136 20.75 20.751 39.860 41.771 1.000 12.49 ANISOU 1020 OE GLU 136 20.75 20.751 39.860 41.771 1.000 12.49 ANISOU 1020 OE1 GLU 136 20.75 20.751 39.860 41.771 1.000 12.49 ANISOU 1020 OE1 GLU 136 20.75 20.751 39.896 41.771 1.000 12.49 ANISOU 1020 OE1 GLU 136 20.75 20.751 39.896 41.771 1.000 12.49 ANISOU 1020 OE1 VAL 137 19.758 19.896 41.771 1.000 12.48 ANISOU 1020 OE1 VAL 137 19.758 19.896 41.771 1.000 12.48 ANISOU 1020 CGL VAL 137 19.758 19.896 41.771 1.000 12.48 ANISOU 1025 CA VAL 137 19.758 19.896 41.771 1.000 12.48 ANISOU 1025 CA VAL 137 19.758 19.607 ANISOU 102 ATOM 1010 CZ ARG 135 14.802 27.184 36.684 1.000 21.69 ANISOU 1010 CZ ARG 135 4004 1906 2333 92 -506 6 4 1011 NH1 ARG 135 14.917 27.843 37.833 1.000 22.26 ATOM ANISOU 1035 CD1 LEU 138 1416 1587 1829 -59 -25 1 7 3 ATOM 1036 CD2 LEU 138 18.052 17.207 37.320 1.000 14.32 ANISOU 1036 CD2 LEU 138 1986 1390 2065 -79 296 370 LEU 138 1986 1390 2065 -/9 296 3 LEU 138 21.903 19.525 37.505 1.000 13.61 LEU 138 1305 2026 1840 -65 174 5 ATOM 1037 C ANISOU 1037 C

ENCOCCID AND SCROOLARS L.

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1038 0
                 LEU 138 22.695 18.760 36.920 1.000 14.97
ANISOU 1038 O
                 LEU 138 1125
                                      2247
                                              2313
                                                       105
                                                             234 178
                       139 22.184 20.816 37.614 1.000 13.26
        1039 N
                  ARG
ANISOU 1039 N
                       139 1432
                  ARG
                                      2046
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                                                       -155 219 317
        1040 CA ARG
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ATOM
ANISOU 1040 CA ARG
                       139 1648
                                      1941
                                              2000
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                                                           502 447
ATOM
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ANISOU 1041 C
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ATOM
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ANISOU 1042 O
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                                     2581
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        1043 CB
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ATOM
                  ARG
ANISOU 1043 CB
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139 24.418 23.487 36.237 1.000 28.66
                  ARG
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MOTA
        1044 CG
                  ARG
ANISOU 1044 CG
                  ARG
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                                              4383
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139 24.245 24.997 36.111 1.000 39.58
        1045 CD
MOTA
                  ARG
ANISOU 1045 CD
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                                                       -3273 119 - 306
                       139 24.910 25.660 37.210 1.000 47.91
        1046 NE
ATOM
                  ARG
ANISOU 1046 NE
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        1047 CZ
ATOM
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ANISOU 1047 CZ
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                                              5802
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ATOM
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ANISOU 1048 NH1 ARG
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ATOM
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ANISOU 1049 NH2 ARG
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                                                      -2746 590 167
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ATOM
        1050 N
                       140 24.562 20.684 39.096 1.000 14.85
                  ALA
                ALA 140 24.502 20.604 57.17 -26 - ALA 140 1287 2204 2151 -517 -26 - ALA 140 25.730 20.257 39.856 1.000 15.80 ALA 140 989 2649 2366 -309 -9 -401 ALA 140 25.444 20.442 41.330 1.000 19.36
ANISOU 1050 N
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        1051 CA
ATOM
ANISOU 1051 CA
ATOM
        1052 CB
ANISOU 1052 CB
                                              2222 243 -435 - 480
ATOM
        1053 C
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ANISOU 1053 C
                  ALA 140 1555
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ALA 140 27.258 18.403 39.796 1.000 18.90
ATOM
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ANISOU 1054 O
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ATOM
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ANISOU 1055 N
                                                      -528 218 -108

    141
    25.340
    16.625
    38.765
    1.000
    15.59

    141
    1256
    2401
    2268
    -192
    -95
    2

    141
    24.207
    15.735
    39.343
    1.000
    14.77

MOTA
        1056 CA
ANISOU 1056 CA
                  THR
                                                      -192 -95 291
       1057 CB
                  THR
ANISOU 1057 CB
                  THR
                       141 1238
                                     2200
                                              2172
                                                      155
                                                             282 3 0 1
                       141 22.946 16.168 38.849 1.000 12.47
       1058 OG1 THR
ANISOU 1058 OG1 THR
                       141 1249
                                              1926
                                     1565
                                                      -31
                                                             295 476
       1059 CG2 THR
                       141 24.167 15.818 40.859 1.000 14.82
ANISOU 1059 CG2 THR
                       141 1394
                                     2077
                                              2160
                                                      135
                                                            -47 177
ATOM
        1060 C
                  THR
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ANISOU 1060 C
                  THR 141 1732
                                     2046
                                              2343
                                                      303
                                                             583
ATOM
        1061 0
                  THR 141 25.432 15.235 36.778 1.000 17.55
ANISOU 1061 O
                  THR
                       141 1991
                                    2104
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                                                             555
ATOM
       1062 N
                       142 25.474 17.416 36.446 1.000 17.74
                  GLY
ANISOU 1062 N
                  GLY
                       142 2127 2197
                                              2416
                                                      303
                                                             260 501
ATOM
        1063 CA
                 GLY
                       142 25.611 17.263 34.987 1.000 17.32
ANISOU 1063 CA
                       142 1642 2494 2447 -160 453 5
142 24.426 16.556 34.358 1.000 16.37
                 GLY
                                                      -160 453 517
ATOM
       1064 C
                  GLY
ANISOU 1064 C
                  GLY
                       142 1619
                                              2710
                                     1893
                                                      261
                                                           472 4 2
ATOM
       1065 O
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                                    15.824 33.379 1.000 18.43
                  GLY
ANISOU 1065 O
                  GLY
                       142 2243
                                     2558
                                                      57 798 1 6 3
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ATOM
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                  THR
                                             34.907 1.000 13.99
ANISOU 1066 N
                       143 1531
                  THR
                                     1429
                                              2356
                                                      83 430 3 5 0
ATOM
       1067 CA
                  THR
                       143 22.049 16.003 34.472
                                                      1.000 14.69
ANISOU 1067 CA
                  THR
                       143 1768
                                     1591
                                              2223
                                                      8
                                                         342.9 3
ATOM
        1068 CB
                  THR
                       143 21.208 15.584 35.700 1.000 15.52
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ANISOU 1068 CB THR 143 1457 1653 2785 55 419 5 2 9 ATOM 1069 OG1 THR 143 22.037 14.784 36.573 1.000 14.63 ANISOU 1069 OG1 THR 143 1296 1792 2471 52 434 3 6 9 1070 CG2 THR 143 20.044 14.738 35.231 1.000 14.24 ANISOU 1070 CG2 THR 143 1761 1981 1669 3 379 1 9 2 1071 C THR 143 21.135 16.785 33.532 1.000 13.96 ANISOU 1071 C THR 143 1553 1708 ANISOU 10/1 C THR 143 1553 1/08 2044 128 4/9 - 1 ATOM 1072 O THR 143 20.642 17.828 33.923 1.000 15.65 ANISOU 1072 O THR 143 2374 1580 1995 315 486 5 ATOM 1073 N GLU 144 20.928 16.279 32.322 1.000 15.32 ANISOU 1073 N GLU 144 1734 1904 2184 -156 260 - 2 ATOM 1074 CA GLU 144 19.917 16.693 31.362 1.000 17.30 ANISOU 1074 CA GLU 144 1686 2470 2417 -377 152 1 CATOM 1075 C GLU 144 18.774 15.693 31.292 1.000 16.84 ANISOU 1075 C GLU 144 18.774 15.693 31.292 1.000 16.84 2044 128 479 -131 1995 315 486 5 5 -156 260 -271 2417 -377 152 1 0 6 ATOM 1075 C GLU 144 18.774 15.693 31.292 1.000 16.84
ANISOU 1075 C GLU 144 1633 2380 2386 -298 313 -2
ATOM 1076 O GLU 144 18.922 14.631 30.680 1.000 16.71
ANISOU 1076 O GLU 144 1470 2057 2821 -43 610 5 8
ATOM 1077 CB GLU 144 2747 3417 2162 -1508 31 - 8
ATOM 1078 CG GLU 144 19.568 17.063 28.825 1.000 37.93
ANISOU 1078 CG GLU 144 19.568 17.063 28.825 1.000 37.93
ANISOU 1078 CG GLU 144 19.293 18.507 28.466 1.000 43.55
ATOM 1079 CD GLU 144 7869 4258 4419 -2497 -2259 2
ATOM 1080 OE1 GLU 144 19.602 19.365 29.326 1.000 51.81
ATOM 1080 OE1 GLU 144 9843 4613 5230 -3180 -832 11
ATOM 1081 OE2 GLU 144 18.766 18.798 27.367 1.000 40.12
ANISOU 1081 OE2 GLU 144 5551 6029 3662 -285 -115 26
ATOM 1082 N PRO 145 17.620 15.959 31.908 1.000 14.29
ANISOU 1082 N PRO 145 1634 1364 2432 -4 208 2 6 5
ATOM 1083 CD PRO 145 17.256 17.136 32.718 1.000 14.14 -298 313 -242 -43 610 5 8 -2057 -2082 1767 -2497 -2259 2129 -3180 -832 1126 -285 -115 2660 1083 CD PRO 145 17.256 17.136 32.718 1.000 14.14 ANISOU 1083 CD PRO 145 1735 1778 1859 32 1 6 7 -55 ATOM 1084 CA PRO 145 16.507 15.000 31.807 1.000 13.72

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ATOM 1086 CG PRO 145 16.132 16.608 33.561 1.000 14.43

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ATOM 1087 C PRO 145 16.076 14.794 30.372 1.000 15.18

ANISOU 1087 C PRO 145 1745 1665 2359 -192 231 287

ATOM 1088 O PRO 145 1745 1665 2359 -192 231 287

ATOM 1088 O PRO 145 16.178 15.685 29.509 1.000 15.40

ANISOU 1088 O PRO 145 2430 1511 1910 -85 613 -15

ATOM 1089 N ASP 146 15.544 13.613 30.070 1.000 15.79

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ATOM 1090 CA ASP 146 14.918 13.366 28.773 1.000 16.74

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ATOM 1094 OD2 ASP 146 6913 5052 3214 16 0 -1182 -323 780 -439 -720 -229 -805 -595 -1282 - 323 146 6913 5052 3214 16 0 -1182 146 13.860 14.441 28.552 1.000 16.65 146 2461 1904 1961 -128 580 -4 146 13.041 14.605 29.457 1.000 15.67 ANISOU 1094 OD2 ASP 1095 C ASP ANISOU 1095 C ASP -128 580 - 40 ATOM 1096 0 ASP ANISOU 1096 O ASP -334 381 -420 147 13.871 15.149 27.429 1.000 20.60 ATOM 1097 N GLY ANISOU 1097 N 147 3484 GLY 2416 1927 -26 419 129 1098 CA GLY 147 12.903 16.212 27.155 1.000 18.06 U 1098 CA GLY 147 2771 2451 1638 -382 98 9 3 ANISOU 1098 CA GLY 147 2771 2451 1638 -382 98 9 3

- 126 -ATOM 1099 C GLY 147 13.361 17.574 27.609 1.000 18.73 ANISOU 1099 C GLY 147 2836 2195 2085 -524 143 52 ATOM 1100 O GLY 147 12.676 18.570 27.282 1.000 18.34 ANISOU 1100 O GLY 147 2865 2416 1687 -413 -72 38 ATOM 1101 N GLY 148 14.498 17.634 28.316 1.000 16.35 -524 143 527 -413 -72 389 1101 N GLY 148 2936 1506 1772 -157 142 8 1102 CA GLY 148 15.116 18.889 28.747 1.000 15.34 ANISOU 1101 N -157 142 8 8 ATOM ANISOU 1102 CA GLY 148 2723 1279 1829 55 450 - 26 GLY 148 14.768 19.339 30.144 1.000 12.97 ATOM 1103 C ATOM 1103 C GLY 148 14.768 19.339 30.144 1.000 12.97
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ANISOU 1106 CA VAL 149 1333 1390 1765 54 -92 1 2 9
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ANISOU 1107 CB VAL 149 1136 1696 1717 -100 246 1 -62 4 0 7 -164 88 3 2 3 155 -31 238 ANISOU 1107 CB VAL 149 1136 1107 CB VAL 149 1136 1696 1717 -100 246 1 1108 CG1 VAL 149 16.358 22.336 33.802 1.000 15.26 -100 246 124 ANISOU 1108 CG1 VAL 149 1941 1922 1936 -195 55 -223 ANISOU 1109 CG2 VAL 149 17.868 20.794 32.538 1.000 17.21 ANISOU 1109 CG2 VAL 149 1231 2045 3265 45 102 -103 ATOM 1110 C VAL 149 14.101 21.482 32.280 1.000 11.32 ATOM 1111 O VAL 149 1186 1303 1813 -78 131 4 7 9 ATOM 1111 O VAL 149 1664 1423 1608 -71 229 16 7 ANISOU 1111 O VAL 149 1664 1423 1608 -71 229 16 7 ANISOU 1112 N GLU 150 13.752 22.463 31.460 1.000 11.96 ANISOU 1113 CA GLU 150 13.47 1453 1746 29 -36 42 0 ATOM 1113 CA GLU 150 12.592 23.286 31.815 1.000 10.90 ANISOU 1113 CA GLU 150 12.592 23.286 31.815 1.000 10.90 ANISOU 1114 CB GLU 150 12.608 24.601 30.999 1.000 17.60 ANISOU 1115 CG GLU 150 13.811 25.488 31.314 1.000 17.86 ANISOU 1115 CG GLU 150 13.811 25.488 31.314 1.000 17.86 ANISOU 1116 CD GLU 150 13.811 25.488 31.314 1.000 17.86 ANISOU 1116 CD GLU 150 3035 13.956 25.929 32.738 1.000 19.47 ANISOU 1116 CD GLU 150 3018 1353 3027 -97 -84 6 6 2 ATOM 1117 OE1 GLU 150 3035 1512 2373 -178 -321 5 3 6 ANISOU 1117 OE1 GLU 150 3035 1512 2373 -178 -321 5 3 6 ANISOU 1118 OE2 GLU 150 3035 1512 2373 -178 -321 5 3 6 ANISOU 1118 OE2 GLU 150 15.109 26.237 33.122 1.000 22.59 ANISOU 1108 CG1 VAL 149 1941 1922 150 15.109 26.237 33.122 1.000 22.59 1118 OE2 GLU ANISOU 1118 OE2 GLU 150 2993 1664 3927 -38 -150 2 8 4 150 11.277 22.533 31.705 1.000 12.22 ATOM 1119 C GLU ANISOU 1119 C GLU GLU 150 1429 1676 1540 235 147 - 5 GLU 150 1429 GLU 150 10.341 22.757 32.530 1.000 13.44 GLU 150 1739 1474 1894 315 470 2 ATOM 1120 O ALA 151 1783 1255 1477 288 ALA 151 1783 1255 1477 288 ANISOU 1120 O ATOM 1121 N ANISOU 1121 N 94 45 253 ATOM 1122 CA ANISOU 1122 CA -100 -413 3 9 6 1123 CB ATOM ANISOU 1123 CB 1851 22 - 269 - 35 ATOM 1124 C ANISOU 1124 C ATOM 1125 0 ANISOU 1125 O -242 204 -108 ATOM 1126 N ANISOU 1126 N 152 1598 152 1598 1259 1598 120 9 2 7 1 152 10.890 18.554 33.602 1.000 10.61 ATOM 1127 CA PHE ANISOU 1127 CA 152 1444 PHE 1061 1526 -33 34 1 6 0 152 1444 1061 1526 -33 34 1 6 0 152 12.293 17.981 33.820 1.000 10.23 1128 CB PHE ANISOU 1128 CB PHE 152 1317 1132 1437 -144 207 410 ATOM 1129 CG 152 12.517 17.187 35.095 1.000 10.36 PHE

- 127 -ANISOU 1129 CG PHE 152 1388 1149 1399 -34 147 276 ATOM 1130 CD1 PHE 152 12.036 15.896 35.229 1.000 11.24 ANISOU 1130 CD1 PHE 152 1479 1047 1743 114 -103 5 114 -103 5 6 6 ATOM 1131 CD2 PHE 152 13.229 17.701 36.154 1.000 11.21 ANISOU 1131 CD2 PHE 152 1489 1449 1319 85 174 1 5 1 1132 CE1 PHE 152 12.252 15.163 36.380 1.000 10.80 ANISOU 1132 CE1 PHE 152 1400 1234 1467 ANISOU 1132 CE1 PHE 152 1400 1234 1467 249 -111 3 7 3 ATOM 1133 CE2 PHE 152 13.431 16.992 37.341 1.000 11.82 ANISOU 1133 CE2 PHE 152 1709 1622 1160 -276 414 2 5 0 ATOM 1134 CZ PHE 152 12.932 15.717 37.457 1.000 11.97 ANISOU 1135 C PHE 152 1651 1604 1293 -255 296 1 7 0 ATOM 1135 C PHE 152 1754 1168 1730 -10 339 8 4 ATOM 1136 O PHE 152 1754 1168 1730 -10 339 8 4 ATOM 1137 N LEU 153 10.809 20.575 34.997 1.000 11.49 ANISOU 1137 N LEU 153 10.809 20.575 34.997 1.000 11.86 ATOM 1138 CA LEU 153 10.532 21.386 36.155 1.000 11.99 ANISOU 1138 CA LEU 153 1890 1229 1437 -165 307 8 5 ATOM 1139 CB LEU 153 1890 1229 1437 -165 307 8 5 ATOM 1139 CB LEU 153 13.059 21.910 36.592 1.000 12.81 ATOM 1140 CG LEU 153 13.059 21.910 36.592 1.000 12.87 ANISOU 1141 CD1 LEU 153 13.059 21.910 36.592 1.000 12.87 ANISOU 1141 CD1 LEU 153 13.185 21.158 37.914 1.000 15.99 ANISOU 1141 CD1 LEU 153 13.185 21.158 37.914 1.000 15.99 ANISOU 1142 CD2 LEU 153 13.185 21.158 37.914 1.000 15.99 ANISOU 1143 C LEU 153 3091 2462 ATOM 1144 CD LEU 153 3091 2462 ATOM 1144 CD LEU 153 3091 2462 ANISOU 1144 CD LEU 153 1667 22.084 36.123 1.000 12.96 ANISOU 1144 CD LEU 153 167 28.084 36.123 1.000 12.96 ANISOU 1144 CD LEU 153 167 3091 2462 ANISOU 1144 CD LEU 153 167 3091 2462 ANISOU 1144 CD LEU 153 167 3091 2462 ANISOU 1144 CD LEU 153 1617 300 22.506 37.193 1.000 13.24 ANISOU 1145 N ASP 154 8.568 22.203 34.955 1.000 13.29 ANISOU 1145 N ASP 154 8.568 22.203 34.955 1.000 13.29 ANISOU 1145 N ASP 154 8.568 22.203 34.955 1.000 13.29 ANISOU 1145 N ASP 154 8.568 22.203 34.955 1.000 13.29 249 -111 3 7 3 1133 CE2 PHE 152 13.431 16.992 37.341 1.000 11.82 ATOM ANISOU 1144 O LEU 153 1617 1302 2109 =443 481 -182 ATOM 1145 N ASP 154 8.568 22.203 34.955 1.000 13.29 ANISOU 1145 N ASP 154 1643 1457 1951 60 517 2 8 0 ATOM 1146 CA ASP 154 7.195 22.671 34.764 1.000 14.21 ANISOU 1145 N ASP 154 1643
ATOM 1146 CA ASP 154 7.195
ANISOU 1146 CA ASP 154 1862
ATOM 1147 CB ASP 154 6.995
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ATOM 1148 CG ASP 154 5.534
ANISOU 1148 CG ASP 154 2323
ANISOU 1149 OD1 ASP 154 2323
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ATOM 1150 OD2 ASP 154 2164
ATOM 1150 OD2 ASP 154 5.168
ANISOU 1150 OD2 ASP 154 6.294
ANISOU 1151 C ASP 154 6.294
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ANISOU 1152 O ASP 154 6.4043
ANISOU 1153 N CYS 155 5.891
ANISOU 1154 CA CYS 155 1425
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ANISOU 1158 O CYS 155 3.215 20.645 37.064 1.000 11.61
ATOM 1159 N GLE 156 4 22 155 1349 1300 156 4.021 19.033 1363 1495 ANISOU 1159 N GLU 156 1263

PRIEDCOID AND SOSSESSES .

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1160 CA
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                 GLU
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ARG 162 4379 2437 4139 -181 332 -1 ANISOU 1219 CD ATOM 1220 NE ANISOU 1220 NE ARG 162 4379 -181 332 -177

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                TYR
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- 131 -ANISOU 1251 CB PRO 165 3640 6479 4227 -1488 380 - 717 ATOM 1252 CG PRO 165 -5.417 20.048 66.569 1.000 36.16 ANISOU 1252 CG PRO 165 3341 6449 3948 -518 -349 --518 -349 - 398 1253 CD PRO 165 -4.197 19.816 65.734 1.000 35.70 ANISOU 1253 CD PRO 165 3440 6296 3828 -1656 -5 -604 ATOM 1254 N LEU 178 4.459 8.087 66.987 1.000 36.23 ANISOU 1254 N LEU 178 4509 3338 5918 -26 1216 1175 ATOM 1254 N LEU 178 4.459 8.087 66.987 1.000 36.23 ANISOU 1254 N LEU 178 4509 3338 5918 -26 1216 1175 ATOM 1255 CA LEU 178 4.994 9.117 66.116 1.000 28.63 ANISOU 1255 CA LEU 178 3397 3170 4312 377 1344 4 0 1 ATOM 1256 CB LEU 178 3497 3245 4688 760 752 -620 ATOM 1257 CG LEU 178 3497 3245 4688 760 752 -620 ATOM 1257 CG LEU 178 3557 2950 4674 667 371 -979 ATOM 1258 CD1 LEU 178 7.859 7.367 64.073 1.000 32.13 ANISOU 1258 CD1 LEU 178 2972 4524 4713 586 810 -790 ATOM 1259 CD2 LEU 178 5303 3695 6850 356 -1656 -1154 ANISOU 1259 CD2 LEU 178 3.885 9.909 65.420 1.000 27.18 ANISOU 1260 C LEU 178 2107 3534 4686 -175 1776 8 3 ATOM 1261 O LEU 178 2.845 9.351 65.086 1.000 39.60 ANISOU 1261 O LEU 178 2407 4624 8016 -1253 1290 2183 ANISOU 1262 N ARG 179 2220 3437 4089 -216 878 74 1 ANISOU 1263 CA ARG 179 3.231 11.973 64.321 1.000 25.04 ANISOU 1263 CA ARG 179 3.231 11.973 64.321 1.000 25.04 ANISOU 1264 C ARG 179 3.231 11.973 64.321 1.000 25.04 ANISOU 1265 O ARG 179 2158 2721 4434 39 99 - 8 9 ATOM 1265 O ARG 179 2158 2721 4434 39 99 - 8 9 ATOM 1265 O ARG 179 2545 3242 5079 441 -332 - 256 ATOM 1266 CB ARG 179 3.517 13.480 64.451 1.000 28.58 ANISOU 1266 CB ARG 179 3980 3317 3561 -110 -843 5 7 ATOM 1267 CG ARG 179 3980 317 3725 3862 57 -957 -3.72 ANISOU 1266 CB ARG 179 3980 3317 3561 -110 -843 5 7
ATOM 1267 CG ARG 179 2.936 14.092 65.724 1.000 30.01
ANISOU 1267 CG ARG 179 3817 3725 3862 57 -957 -3.72
ATOM 1268 CD ARG 179 3.307 15.570 65.757 1.000 31.51
ANISOU 1268 CD ARG 179 4457 3675 3840 90 -1514 -3 3 8
ATOM 1269 NE ARG 179 2.925 16.126 67.058 1.000 37.82
ANISOU 1269 NE ARG 179 7035 3190 4144 153 -310 - 1 5
ATOM 1270 CZ ARG 179 2.897 17.425 67.292 1.000 39.43
ANISOU 1270 CZ ARG 179 8420 3029 3532 -479 580 4 0 0
ATOM 1271 NH1 ARG 179 3.213 18.286 66.331 1.000 59.73
ANISOU 1271 NH1 ARG 179 11745 4676 6273 -1045 3177 1.72 2
ATOM 1272 NH2 ARG 179 2.548 17.896 68.457 1.000 33.13
ANISOU 1272 NH2 ARG 179 5661 3832 3094 275 -1463 -173
ATOM 1273 N MET 180 4.455 11.099 62.424 1.000 21.43
ANISOU 1273 N MET 180 2013 2457 3674 -395 108 -222
ATOM 1274 CA MET 180 4.695 10.539 61.108 1.000 20.07
ANISOU 1274 CA MET 180 2346 1965 3315 -349 -300 1 5 1 ANISOU 1274 CA MET 180 2346 1965 3315 -349 -300 1 5 1 1274 CA MET 180 2346 1965 3315 -349 -300 1 3 1275 C MET 180 5.802 9.482 61.182 1.000 17.33 1275 C MET 180 2251 2080 2254 -332 -86 3 3 1276 O MET 180 6.894 9.757 61.677 1.000 18.52 1276 O MET 180 2237 2019 2781 -398 -79 5 2 1277 CB MET 180 5.041 11.646 60.136 1.000 22.64 1277 CB MET 180 2571 2321 3709 -197 -549 6 8 ANISOU 1275 C ATOM 1276 O -332 -86 337 ANISOU 1276 O MOTA 180 2571 2321 3709 -197 -549 6 8 3 180 5.065 11.367 58.678 1.000 27.90 180 3918 3095 3588 -453 -654 9 1 3 ANISOU 1277 CB MET 1278 CG MET ATOM ANISOU 1278 CG MET ATOM 1279 SD MET 180 4.945 12.838 57.629 1.000 25.01 ANISOU 1279 SD MET 180 2936 2942 3626 -399 124 8 -399 124 851 1280 CE MET 180 4.385 12.010 56.147 1.000 37.00 ANISOU 1280 CE MET 180 5917 3450 4690 -258 -2680 1204 ATOM 1281 N ALA 181 5.467 8.295 60.680 1.000 16.99 ANISOU 1281 N ALA 181 2144 2139 2174 -90 -558 2 9 9

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- 132 -
ATOM
       1282 CA
                ALA 181 6.396
                                  7.168 60.676 1.000 16.12
ANISOU 1282 CA
                ALA
                                  1958 1890 -171 -343 6
5.891 60.279 1.000 20.24
                     181 2275
                                                 -171 -343602
ATOM
       1283 CB
                     181 5.668
                ALA
                     181 2857
ANISOU 1283 CB
                ALA
                                  2158
                                          2673
                                                 -648 694 106
       1284 C
                     181 7.576
                ALA
                                  7.409
                                          59.738 1.000 15.43
ANISOU 1284 C
                     181 2223
                ALA
                                 1717
                                          1925
                                                 -315 -369 4 3 2
ATOM
       1285 0
                ALA
                    181 7.458
                                8.198
                                          58.783
                                                 1.000 15.49
ANISOU 1285 O
                ALA
                     181 2268
                                 1761
                                          1858
                                                 -173 -296 4 3 4
ATOM
                     182 8.698 6.733
       1286 N
                PRO
                                        59.986 1.000 16.03
ANISOU 1286 N
                PRO 182 2517
                                 1745
                                          1829
                                                 32 - 78 5 3 1
ATOM
       1287 CD
                PRO
                    182 8.983
                                5.802 61.101 1.000 19.61
ANISOU 1287 CD
                PRO
                     182 2321
                                 2908
                                          2221
                                                 -210 -306 1 2 4 0
                PRO
       1288 CA
                     182 9.865 6.907
                                        59.076 1.000 14.78
ANISOU 1288 CA
                PRO
                     182 2573
                                 1336
                                         1706
                                                 -101 -86 299
                     182 10.914 5.948 59.649 1.000 16.20 182 2570 1978 1607 170 -251 7
                     182 2570 1978 1607 170 -251 7
182 10.479 5.713 61.066 1.000 19.28
182 2301 3071 1952 -199
ATOM
       1289 CB
                PRO
ANISOU 1289 CB
                PRO
                                                       -251 7 7
       1290 CG
ATOM
                PRO
ANISOU 1290 CG PRO
                                                 -199 -245 1 0 0 1
       1291 C
                PRO
                     182 9.541
                                6.J.
1658
                                  6.571
                                          57.627 1.000 14.90
ANISOU 1291 C.
               PRO
                     182 2230
                                          1772
                                                 -421 -262 3 4 0
ATOM
       1292 0
                PRO
                                          57.249
                     182 8.920 5.573
                                                1.000 15.38
ANISOU 1292 O
                PRO
                     182 2301
                                          1957
                                 1587
                                                 -467 - 482539
ATOM
       1293 N
                     183 9.969 7.460 56.730 1.000 12.28
                HIS
ANISOU 1293 N
                HIS
                     183 1737
                                1312
                                         1617
                                                 -154 -284 1 5 6
ATOM
       1294 CA
                HIS
                     183 9.733 7.354
                                        55.300 1.000 11.90
ANISOU 1294 CA
                HIS
                                1495 1614 -254 -351 3
7.824 54.922 1.000 12.43
                     183 1413
                                                 -254 -351 3
ATOM
       1295 CB
                HIS
                                1368 1957
9.314 55.08
                     183 8.300
ANISOU 1295 CB
                HIS
                     183 1399
                                                 -128 -241 1 1 2
       1296 CG
                HIS
                     183 8.168
                                        55.089 1.000 11.36
ANISOU 1296 CG HIS
                                1369 1600 -367 -296 5
10.374 54.249 1.000 12.03
1296 1589 -43 157 -
                     183 1349
                                                 -367 -296 5 6
ATOM
       1297 CD2 HIS
                     183 8.259
ANISOU 1297 CD2 HIS
                     183 1684
                                                 -43 157 - 10
                     183 7.989 9.858
ATOM
       1298 ND1 HIS
                                          56.339 1.000 13.27
ANISOU 1298 ND1 HIS
                     183 1901
                                 1439
                                          1700
                                                 -65 267 193
                    183 7.943 11.187 56.244 1.000 12.43
       1299 CE1 HIS
ATOM
ANISOU 1299 CE1 HIS
                     183 1939
                                 1490
                                          1296
                                                 77 -244 150
       1300 NE2 HIS
ATOM
                    183 8.101 11.515 54.992 1.000 11.04
ANISOU 1300 NE2 HIS
                     183 1560
                     183 1560 1437
183 10.749 8.176
                                          1199
                                                 215 -232 4 8
ATOM
       1301 C
                HIS
                                        54.515 1.000 12.27
ANISOU 1301 C
                HIS
                     183 1446 1639 1577 -303 -282 -
183 11.433 9.032 55.064 1.000 12.94
                                                  -303 -282 - 67
ATOM
       1302 0
                                        1505
53
                HIS
ANISOU 1302 O
                     183 1496
                HIS
                                  1915
                                                 -558 -292 1 5
                TYR 184 10.849 7.907
ATOM
       1303 N
                                          53.215 1.000 10.61
ANISOU 1303 N
                TYR 184 1453
                                  1027
                                          1552
                                                 -41
                                                       -380 1 1 0
       1304 CA TYR
ATOM
                    184 11.483 8.800
                                          52.256 1.000 11.36
ANISOU 1304 CA
                    184 1475
               TYR
                                  1104
                                          1738
                                                 -71
                                                       -264 1 7 8
       1305 CB
ATOM
                TYR
                     184 12.628 8.151
                                          51.481 1.000 11.79
ANISOU 1305 CB
                TYR
                     184 1631
                                 1114
                                          1734
                                                 -62
                                                      -197 3 4
                     184 12.368 6.907 50.677 1.000 11.29
       1306 CG
ATOM
                TYR
ANISOU 1306 CG
                TYR
                     184 1680 921 1688 225 -893 174
       1307 CD1 TYR
ATOM
                     184 12.156 5.659 51.268 1.000 11.76
ANISOU 1307 CD1 TYR
                     184 1663 927 1879 388 -487 190
184 11.911 4.526 50.492 1.000 12.64
                                                    -487 190
       1308 CE1 TYR
ANISOU 1308 CE1 TYR
                     184 1960 878 1964 173 -40 182
184 12.333 6.949 49.279 1.000 11.13
       1309 CD2 TYR
ANISOU 1309 CD2 TYR
                     184 1252
                                  1302
                                          1674
                                                  109 -283 9 3
                     184 1252 1302
184 12.102 5.834
       1310 CE2 TYR
                                         48.502 1.000 12.93
ANISOU 1310 CE2 TYR
                     184 1944
                                  1422
                                          1546
                                                  49 - 384 7 3
                     184 11.898 4.611
       1311 CZ
                 TYR
                                          49.121 1.000 13.14
ANISOU 1311 CZ
                     184 1717 1304
184 11.663 3.490
                 TYR
                                          1972
                                                  30 -611 6 7
       1312 OH
                                        48.343 1.000 15.45
MOTA
                TYR
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- 133 -ANISOU 1312 OH TYR 184 2028 1471 2373 42 -476 - 247 ATOM 1313 C TYR 184 10.447 9.390 51.314 1.000 11.50 ANISOU 1313 C TYR 184 1445 1215 1709 -187 -201 3 4 8 ATOM 1314 O TYR 184 9.362 8.797 51.089 1.000 11.75 ANISOU 1314 O TYR 184 1305 1308 1853 -106 -171 4 2 3 -187 -201 3 4 8 -171 4 2 7 1315 N ASP 185 10.784 10.557 50.743 1.000 10.79 1315 N ASP 185 1581 1069 1449 -141 -132 1 ANISOU 1315 N -141 -132 1 1 8 1316 CA ASP 185 9.861 11.218 49.815 1.000 9.10 ANISOU 1316 CA ASP 185 1089 1093 1277 -326 23 2 0 6
ATOM 1317 CB ASP 185 9.934 12.743 49.886 1.000 10.13
ANISOU 1317 CB ASP 185 1427 1095 1327 -298 -178 1 7 7
ATOM 1318 CG ASP 185 9.540 13.388 51.185 1.000 11.79
ANISOU 1318 CG ASP 185 1797 1350 1333 -250 -149 1 1
ATOM 1319 OD1 ASP 185 9.681 14.638 51.278 1.000 13.79
ANISOU 1319 OD1 ASP 185 2050 1316 1875 135 -52 - 2 6
ATOM 1320 OD2 ASP 185 9.114 12.755 52.189 1.000 13.31
ANISOU 1320 OD2 ASP 185 1805 1848 1405 -411 -63 1 0 5
ATOM 1321 C ASP 185 10.098 10.759 48.371 1.000 9.44
ANISOU 1322 O ASP 185 11.234 10.469 48.005 1.000 10.64
ANISOU 1322 O ASP 185 11.234 10.469 48.005 1.000 10.64
ANISOU 1322 O ASP 185 11.234 10.469 48.005 1.000 10.64 ANISOU 1316 CA ASP 185 1089 1093 1277 -326 23 2 0 6 ANISOU 1322 O ASP 185 1167 1376 1500 -127 -35 -ATOM 1323 N LEU 186 9.038 10.684 47.568 1.000 10.09 -127 -35 -206 ATOM 1323 N LEU 186 9.038 10.684 47.568 1.000 10.09 ANISOU 1323 N LEU 186 1211 1186 1437 -272 -177 - 5 ATOM 1324 CA LEU 186 9.124 10.312 46.161 1.000 10.60 ANISOU 1324 CA LEU 186 1641 986 1401 -239 -52 - 44 ATOM 1325 CB LEU 186 8.030 9.295 45.798 1.000 11.32 ANISOU 1325 CB LEU 186 1652 929 1721 -111 17 -479 ATOM 1326 CG LEU 186 7.989 7.977 46.602 1.000 12.60 ANISOU 1326 CG LEU 186 1408 1039 2340 -263 -200 - 1 ATOM 1327 CD1 LEU 186 6.896 7.064 46.028 1.000 16.64 ANISOU 1327 CD1 LEU 186 9.356 7.064 46.028 1.000 16.64 ANISOU 1328 CD2 LEU 186 9.356 7.332 46.629 1.000 13.84 ANISOU 1328 CD2 LEU 186 1438 1245 2575 -155 443 28 ATOM 1329 C LEU 186 9.024 11.521 45.223 1.000 10.90 1437 -272 -177 - 58 -263 -200 - 166 -634 -398 - 135 -155 443 283 ATOM 1329 C LEU 186 9.024 11.521 45.223 1.000 10.90 ANISOU 1329 C LEU 186 1327 1211 1603 -3 -451 164 ATOM 1330 O LEU 186 8.768 11.406 44.031 1.000 13.60 ANISOU 1330 O LEU 186 2067 1608 1494 -211 -321 103 ATOM 1331 N SER 187 9.264 12.705 45.734 1.000 10.71 ANISOU 1331 N SER 187 1546 1129 1393 -76 -282 3 1 8 ATOM 1332 CA SER 187 9.401 13.943 44.998 1.000 10.49 ANISOU 1332 CA SER 187 1427 1191 1370 195 -107 4 8 8 ATOM 1333 CB SER 187 9.221 15.103 46.002 1.000 10.56 ANISOU 1333 CB SER 187 1105 1048 1857 298 161 5 3 2 ATOM 1334 OG SER 187 10.430 14.918 46.726 1.000 13.01 ANISOU 1334 OG SER 187 10.430 14.918 46.726 1.000 13.01 ANISOU 1335 C SER 187 10.774 14.062 44.336 1.000 10.47 ANISOU 1335 C SER 187 10.774 14.062 44.336 1.000 10.47 ANISOU 1335 C SER 187 1447 862 1669 135 -3 1 4 5 ATOM 1335 C SER 187 1447 862 1669 135 -3 1 4 5 ATOM 1336 O SER 187 11.684 13.246 44.513 1.000 10.54 1329 C LEU 186 9.024 11.521 45.223 1.000 10.90 1336 O SER 187 11.684 13.246 44.513 1.000 10.54 MOTA ANISOU 1336 O SER 187 1577 799 1629 183 -91 - 77 1337 N MET 188 10.962 15.095 43.502 1.000 9.78 MOTA ANISOU 1337 N MET 188 1419 978 1318 147 44 7 4 ATOM 1338 CA MET 188 12.267 15.584 43.065 1.000 9.94 MET ANISOU 1338 CA 188 1394 942 1441 182 58 3 7 ATOM 1339 CB MET ANISOU 1339 CB MET ATOM 1340 CG MET 188 13.363 17.23 ANISOU 1340 CG MET 188 1403 1172 1756 46 -51 2 1 4 ATOM 1341 SD MET 188 14.687 16.134 40.891 1.000 12.71 ANISOU 1341 SD MET 188 1619 1272 1940 139 137 1 ATOM 1342 CE MET 188 16.061 17.267 40.790 1.000 13.86 139 137 198

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- 134 -
ATOM
       1343 C
                MET
                      188 12.946 16.217 44.291 1.000 12.13
ANISOU 1343 C
                      188 1325
                MET
                                  1586
                                          1698
                                                  169
                                                       -18 -285
MOTA
       1344 0
                MET
                      188 13.971
                                  15.727
                                          44.804 1.000 11.52
ANISOU 1344 O
                MET
                      188 1288
                                  1553
                                          1535
                                                  144
                                                       132 8 7
       1345 N
                VAL
                      189 12.362
                                  17.290
                                          44.838 1.000 10.00
ANISOU 1345 N
                VAL
                      189 1290
                                  1217
                                          1292
                                                  53 -175 6
ATOM
       1346 CA
                VAL
                      189 12.745
                                  17.894
                                          46.099 1.000 9.70
ANISOU 1346 CA
                VAL
                      189 1209
                                  1057
                                          1420
                                                  -212 -45 -19
MOTA
       1347 CB
                     189 13.618 19.154 45.979
                VAL
                                                  1.0009.97
ANISOU 1347 CB
                VAL 189 1288
                                  1103
                                          1398
                                                  -238 129 189
                    189 14.953 18.837 45.266 1.000 13.45
ATOM
       1348 CG1 VAL
ANISOU 1348 CG1 VAL
       1349 CG2 VAL 189 1334 1410 2368 -236 390 143 1349 CG2 VAL 189 12.899 20.289 45.264 1.000 12.24 1349 CG2 VAL 189 1715 1242 1693 -25 150 295 1350 C VAL 189 11.469 18.245 46.871 1.000 10.10 1350 C VAL 189 1089 1600 1149 -456 -156 - 73 1351 O VAL 189 10.405 18 399 46 350
MOTA
ANISOU 1349 CG2 VAL
MOTA
ANISOU 1350 C
ATOM
                     189 10.405 18.399 46.250 1.0J0 9.53
ANISOU 1351 O
                VAL
                     189 1153
                                  1249
                                          1217
                                                  -222 -190 8
ATOM
       1352 N
                     190 11.609
                THR
                                 18.327 48.187 1.000 8.66
ANISOU 1352 N
                THR
                     190 1273
                                  894 1123
                                              15 -202 127
ATOM
       1353 CA
                     190 10.565 18.771 49.091 1.000 9.64
               THR
ANISOU 1353 CA
               THR
                     190 1350
                                  1167
                                          1147
                                                  -11
                                                        -228 - 99
ATOM
       1354 CB
               THR
                     190 10.194 17.699 50.132 1.000 10.69
ANISOU 1354 CB THR
                     190 1231
                                  1196
                                          1635
                                                        121 - 54
                                                  -300
       1355 OG1 THR
ATOM
                     190 9.662
                                  16.586 49.501 1.000 12.45
ANISOU 1355 OG1 THR
                     190 1333
                                  1341
                                          2055
                                                  -140 -258 - 48
ATOM
       1356 CG2 THR
                     190 9.038
                                 18.131 51.019 1.000 13.59
ANISOU 1356 CG2 THR
                     190 1121
                                  2222
                                          1821
                                                  -272 151 -195
       1357 C
ATOM
                     19.0 11.058 19.976 49.891 1.000 9.23
190 1257 1096 1152 -102 -336 -
                THR
ANISOU 1357 C
                THR
                                  1096
                                          1152
                                                  -102 -336 - 49
ATOM
       1358 0
                     190 12.149
                                 19.867 50.447 1.000 10.54
                THR
ANISOU 1358 O
                THR
                     190 1322
                                  1292
                                                  -5 -359 -122
                                          1390
ATOM
       1359 N
                                 21.064 49.978 1.000 10.23
                LEU
                     191 10.313
ANISOU 1359 N
                     191 1319
                LEU
                                  1167
                                          1401
                                                  -71 -177 -133
ATOM
       1360 CA
                     191 10.691 22.241 50.770 1.000 10.19
               LEU
ANISOU 1360 CA
               LEU
                     191 1259
                                  1176
                                          1438
                                                  0 - 294 - 142
MOTA
       1361 CB
                LEU
                     191 10.604 23.511 49.910 1.000 11.52
ANISOU 1361 CB
                LEU
                     191 1203
                                  1185
                                          1990
                                                  -118 -601 3 2
       1362 CG
ATOM
                     191 11.897 23.898 49.167 1.000 13.23
                LEU
ANISOU 1362 CG
                LEU
                     191 1898
                                  1710
                                          1419
                                                  -391 -3589 7
       1363 CD1 LEU
                     191 12.333 22.794 48.218 1.000 15.25
ANISOU 1363 CD1 LEU
                     191 1685
                                  2018
                                          2091
                                                  -476 -214 -305
       1364 CD2 LEU
                     191 11.717 25.231 48.448 1.000 17.46
ANISOU 1364 CD2 LEU
                     191 2310
                                  2044
                                          2281
                                                  -14
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ATOM
       1365 C
                LEU
                     191 9.798
                                  22.328 52.006 1.000 11.93
ANISOU 1365 C
                LEU
                     191 1275
                                  1677
                                          1579
                                                  56 - 190 - 372
ATOM
       1366 0
                LEU
                     191 8.560
                                  22.262
                                          51.868 1.000 13.49
ANISOU 1366 O
                LEU
                     191 1276
                                  2173
                                          1676
                                                  1 -192 -601
ATOM
       1367 N
                ILE
                     192 10.394 22.483
                                          53.190 1.000 11.06
ANISOU 1367 N
                ILE
                     192 1115
                                  1603
                                          1487
                                                  -111 -92 -108
ATOM
                ILE
       1368 CA
                     192 9.671
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ANISOU 1368 CA
                     192 1071
                ILE
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                                                  11 -173 -149
ATOM
       1369 CB
                ILE
                     192 9.927
                                  21.304 55.330 1.000 12.94
ANISOU 1369 CB
                ILE
                     192 2099
                                  1586
                                          1232
                                                  -65
       1370 CG2 ILE
                     192 9.221
                                  21.428 56.673 1.000 16.06
ANISOU 1370 CG2 ILE
                      192 2479
                                  1983
                                          1641
                                                  -206 426 -215
       1371 CG1 ILE
ATOM
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                                  20.028 54.590 1.000 15.51
ANISOU 1371 CG1 ILE
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                                  1658
                                          1601
                                                  -400 -48 -175
       1372 CD1 ILE
ATOM
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                                  18.765 55.339 1.000 25.71
ANISOU 1372 CD1 ILE
                      192 5869
                                  1608
                                          2290
                                                  -175 -1566 -301
ATOM
       1373 C
                ILE
                      192 9.966
                                  23.809 55.253 1.000 11.47
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ANISOU 1373 C ILE 192 1330 1603 1427 -4 -222 -12
ATOM 1374 O ILE 192 11.123 24.106 55.567 1.000 13.33
ANISOU 1374 O ILE 192 1344 1738 1981 -96 -289 -2
ATOM 1375 N GLN 193 8.904 24.525 55.602 1.000 15.78
ANISOU 1375 N GLN 193 1316 2462 2219 -64 -5 -97
ATOM 1376 CA GLN 193 8.987 25.653 56.533 1.000 14.56
ANISOU 1376 CA GLN 193 1582 1858 2091 212 -304 -5
ATOM 1377 CB GLN 193 8.449 26.975 56.020 1.000 20.03
ANISOU 1377 CB GLN 193 8.449 26.975 56.020 1.000 20.03
ANISOU 1377 CB GLN 193 2226 2203 3180 318 -329 14
ATOM 1378 CG GLN 193 9.203 27.684 54.914 1.000 23.86 -4 -222 -122 -96 -289 - 219 -64 -5 -975 -304 - 529 -329 1 4 2 ANISOU 1378 CG GLN 193 3399 2492 3174 313 45 280 ATOM 1379 CD GLN 193 8.665 29.079 54.675 1.000 22.92 ANISOU 1379 CD GLN 193 3250 2363 3097 78 -477 205 ATOM 1380 OE1 GLN 193 7.603 29.292 54.099 1.000 27.68 ATOM 1380 OE1 GLN 193 7.603 29.292 54.099 1.000 27.68 ANISOU 1380 OE1 GLN 193 4175 3310 3031 552 -1214 2 9 ATOM 1381 NE2 GLN 193 9.411 30.075 55.134 1.000 27.01 ANISOU 1381 NE2 GLN 193 3187 2667 4408 -440 124 1 7 ATOM 1382 C GLN 193 8.216 25.265 57.804 1.000 15.14 ANISOU 1382 C GLN 193 1945 1827 1982 136 -174 - 722 ATOM 1383 O GLN 193 7.147 24.662 57.714 1.000 27.80 ANISOU 1383 O GLN 193 2523 6225 1817 -1586 -592 2 3 5 ATOM 1384 N GLN 194 8.714 25.552 58.978 1.000 19.80 ANISOU 1385 CA GLN 194 8.100 25.080 60.213 1.000 22.89 ANISOU 1385 CA GLN 194 3961 2626 2110 493 -20 5 2 GLN 194 3961 2626 2110 493 -20 5 2 GLN 194 7.763 26.236 61.141 1.000 27.79 ANISOU 1385 CA GLN 194 3961 MOTA 1386 C ANISOU 1386 C GLN 194 4886 2757 2916 823 25 - 262
ATOM 1387 O GLN 194 8.424 27.258 60.983 1.000 30.03
ANISOU 1387 O GLN 194 4727 3168 3516 368 -259 - 910
ATOM 1388 CB GLN 194 9.086 24.170 60.950 1.000 23.97
ANISOU 1388 CB GLN 194 3952 3133 2021 846 483 352
ATOM 1389 CG GLN 194 9.398 22.835 60.314 1.000 21.94
ANISOU 1389 CG GLN 194 2740 3238 2358 683 -182 - 1 0
ATOM 1390 CD GLN 194 10.546 22.148 61.052 1.000 20.51
ANISOU 1390 CD GLN 194 2450 3433 1911 509 -321 - 429
ATOM 1391 OE1 GLN 194 11.707 22.142 60.627 1.000 20.80
ANISOU 1392 NE2 GLN 194 2245 2996 2662 -171 -382 - 681
ATOM 1392 NE2 GLN 194 10.223 21.585 62.197 1.000 24.91 ANISOU 1386 C ATOM 1387 O GLN 194 4886 2757 2916 823 25 - 262 1392 NE2 GLN 194 10.223 21.585 62.197 1.000 24.91 ATOM 1392 NE2 GLN 194 10.223 21.585 62.197 1.000 24.91

ANISOU 1392 NE2 GLN 194 2539 3902 3023 210 -365 76 0

ATOM 1393 N THR 195 6.817 26.035 62.030 1.000 32.47

ANISOU 1393 N THR 195 5716 2729 3891 1095 1056 -616

ATOM 1394 CA THR 195 6.588 26.708 63.282 1.000 35.83

ANISOU 1394 CA THR 195 6329 3539 3748 1011 999 -722

ATOM 1395 CB THR 195 5.263 27.492 63.357 1.000 37.96

ANISOU 1395 CB THR 195 5756 4304 4365 647 2095 -1151

ATOM 1396 OG1 THR 195 4.191 26.576 63.604 1.000 48.36

ANISOU 1397 CG2 THR 195 6874 6076 5423 -806 2581 -1842

ATOM 1397 CG2 THR 195 4.958 28.175 62.033 1.000 44.54

ANISOU 1398 C THR 195 6.590 25.684 64.429 1.000 48.86

ANISOU 1398 C THR 195 10133 4924 3508 -321 -1356 -221 ANISOU 1398 C THR 195 10133 4924 3508 -321 -1356 -221 ATOM 1399 0 THR 195 6.122 24.544 64.293 1.000 64.12 1399 O THR 195 6.122 24.544 64.293 1.000 64.12
1399 O THR 195 13267 4150 6945 -264 -4541 1
1400 N PHE 201 12.035 21.374 72.205 1.000 71.12
1400 N PHE 201 13961 9034 4028 -5932 -1658 1401 CA PHE 201 11.775 20.053 71.629 1.000 49.44
1401 CA PHE 201 7918 7543 3326 -3128 1317 -1
1402 CB PHE 201 10.469 19.464 72.181 1.000 47.85
1402 CB PHE 201 7119 6892 4168 -1869 1937 -1
1403 CG PHE 201 10.130 18.113 71.545 1.000 46.41
1403 CG PHE 201 6643 6596 4396 -2038 1879 -1 ANISOU 1399 O -264 -4541 1682 MOTA ANISOU 1400 N -5932 -1658 -1741 ANISOU 1401 CA -3128 1317 -1488 ATOM ANISOU 1402 CB -1869 1937 - 1899 MOTA ANISOU 1403 CG -2038 1879 - 1497

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- 136 -1404 CD1 PHE 201 10.738 16.954 71.991 1.000 50.03 ANISOU 1404 CD1 PHE 201 7982 6634 4393 -2326 1092 - 991 ATOM 1405 CD2 PHE 201 9.220 18.001 70.513 1.000 42.63 ANISOU 1405 CD2 PHE 201 5458 6427 4313 -1097 2449 - 2268 MOTA 1406 CE1 PHE 201 10.434 15.739 71.417 1.000 49.95 ANISOU 1406 CE1 PHE 201 8275 6464 -2047 227 -716 4240 1407 CE2 PHE 201 8.901 16.783 69.934 1.000 41.38 201 9.515 15.636 201 7075 6261 ANISOU 1407 CE2 PHE 3762 -578 2006 - 1844 1408 CZ PHE 15.636 70.392 1.000 44.74 ANISOU 1408 CZ PHE 3663 -1063 1020 - 975 201 11.722 20.110 70.107 1.000 42.42 1409 C ATOM PHE ANISOU 1409 C PHE 201 6324 6442 3351 -1964 717 -1441 201 11.007 20.941 69.536 1.000 47.79 ATOM 1410 0 PHE ANISOU 1410 O PHE 201 9668 4400 201 9668 4400 4090 -762 691 -2416 202 12.477 19.232 69.449 1.000 34.04 1411 N VAL VAL 202 4525 ANISOU 1411 N 5852 2558 -1948 7 -425 ATOM 1412 CA 202 12.535 19.245 67.993 1.000 25.09 VAL ANISOU 1412 CA VAL 202 3221 3752 2558 -1041 -182 9 9 1413 CB **ATOM** 202 13.988 19.286 67.489 1.000 22.88 VAL ANISOU 1413 CB VAL 202 2832 3430 2432 -577 -691 -198 1414 CG1 VAL 202 14.053 19.387 65.965 1.000 26.02 202 3821 3594 2470 -958 35 - 27 - ANISOU 1414 CG1 VAL -958 35 - 277 1415 CG2 VAL 202 14.771 20.443 ATOM 68.078 1.000 24.69 ANISOU 1415 CG2 VAL 202 3043 3473 2867 -786 - 410 - 3201416 C ATOM VAL 202 11.798 18.035 67.421 1.000 20.69 ANISOU 1416 C VAL 202 3027 2810 2023 -648 58 6 1 '5 MOTA 1417 0 VAL 202 12.288 16.914 67.581 1.000 26.08 ANISOU 1417 O VAL 202 3294 3219 3396 -136 452 884 ATOM 1418 N 203 10.662 18.234 66.766 1.000 20.21 SER ANISOU 1418 N SER 203 3100 2794 1787 -414 25 - 152 1419 CA SER ATOM 203 9.820 203 3149 17.192 66.218 1.000 20.37 ANISOU 1419 CA SER 2709 1884 -355 129 -256 1420 CB SER 203 8.437 203 2726 203 7.841 ATOM 17.779 65.896 1.000 24.72 ANISOU 1420 CB SER 4106 2558 -178 369 -1015 ATOM 1421 OG SER 18.239 67.097 1.000 31.80 ANISOU 1421 OG SER 203 3328 -457 1175 -1104 5782 2974 MOTA 1422 C 203 10.367 16.524 64.958 1.000 19.13 SER SER 203 2580 2647 2040 -339 170 -244 SER 203 10.279 15.302 64.832 1.000 17.01 SER 203 2311 2625 1527 -414 206 -18 ANISOU 1422 C ATOM 1423 0 ANISOU 1423 O ATOM 1424 N LEU 204 10.902 17.259 63.998 1.000 16.16 ANISOU 1424 N LEU 204 2142 1976 2024 71 77 - 292 ATOM 1425 CA LEU 204 11.403 16.679 62.740 1.000 14.07 ANISOU 1425 CA LEU 204 1670 1626 2049 -22 -24 -283 1426 CB LEU ATOM 204 11.269 17.704 61.618 1.000 13.80 ANISOU 1426 CB LEU 204 1549 1763 1931 -249 -340 -2771427 CG ATOM LEU 204 11.647 17.272 60.212 1.000 14.13 ANISOU 1427 CG 204 1726 LEU 1722 1919 -253 -482 -412 ATOM 1428 CD1 LEU 204 10.770 16.134 59.680 1.000 18.76 ANISOU 1428 CD1 LEU 204 2579 2895 1654 -1297 -927 -106 1429 CD2 LEU 204 11.609 59.255 1.000 16.20 18.478 ANISOU 1429 CD2 LEU 204 1987 2095 2074 65 75 - 123 1430 C MOTA LEU 204 12.832 16.140 62.885 1.000 14.81 ANISOU 1430 C LEU 204 1734 1748 2144 9 -199 -250 MOTA 1431 0 LEU 204 13.699 16.853 63.397 1.000 15.52 ANISOU 1431 O LEU 204 1833 1789 2274 -59 -435 - 42 ATOM 1432 N 205 13.065 14.900 62.469 1.000 14.42 GLN ANISOU 1432 N GLN 205 1847 1804 1827 189 -120 - 153 1433 CA 205 14.288 14.143 62.574 1.000 12.76 GLN ANISOU 1433 CA GLN 205 1777 1655 1419 43 - 347 - 113 ATOM 1434 C 205 14.622 13.434 61.260 1.000 11.12 GLN

- 137 -ANISOU 1434 C GLN 205 1412 1474 1338 49 -468 - 21
ATOM 1435 O GLN 205 13.707 12.927 60.606 1.000 13.97
ANISOU 1435 O GLN 205 1622 2235 1449 -293 -449 - 14
ATOM 1436 CB GLN 205 14.164 13.062 63.662 1.000 15.57
ANISOU 1436 CB GLN 205 2421 1925 1568 341 151 8 3
ATOM 1437 CG GLN 205 13.863 13.635 65.032 1.000 18.58
ANISOU 1437 CG GLN 205 3321 2286 1451 689 -1298 2 -293 -449 - 147 ANISOU 1437 CG GLN 205 3321 2286 1451 689 -1298 2 ATOM 1438 CD GLN 205 15.086 14.243 65.680 1.000 24.33 ANISOU 1438 CD GLN 205 3687 3465 2091 520 -499 -57 ATOM 1439 OE1 GLN 205 16.206 13.717 65.549 1.000 29.12 ANISOU 1439 OE1 GLN 205 3350 3464 4251 14 -270 -180 520 -499 - 570 ATOM 1449 OE1 GLN 205 16.206 13.717 65.549 1.000 29.12 ANISOU 1440 NE2 GLN 205 3350 3464 4251 14 -270 -1800 ATOM 1440 NE2 GLN 205 3055 2465 3225 335 -592 -140 ANISOU 1440 NE2 GLN 205 3055 2465 3225 335 -592 -140 ATOM 1441 N ALA 206 15.893 13.401 60.893 1.000 12.63 ANISOU 1441 N ALA 206 1523 1770 1506 -251 -234 - 6 ATOM 1442 CA ALA 206 16.335 12.649 59.731 1.000 13.77 ANISOU 1442 CA ALA 206 16.693 13.519 58.528 1.000 16.34 ANISOU 1443 CB ALA 206 16.693 13.519 58.528 1.000 16.34 ANISOU 1444 C ALA 206 17.567 11.813 60.046 1.000 15.92 ATOM 1444 C ALA 206 1489 2331 2230 -290 179 -341 ATOM 1445 O ALA 206 18.368 12.182 60.908 1.000 15.86 ANISOU 1446 N GLU 207 17.707 10.712 59.305 1.000 16.98 ANISOU 1446 N GLU 207 1981 2086 2383 -335 348 -186 ATOM 1447 CA GLU 207 1981 2086 2383 -335 348 -186 ATOM 1444 C GLU 207 18.938 9.942 59.364 1.000 20.58 ANISOU 1448 C GLU 207 18.938 9.942 59.364 1.000 20.58 ANISOU 1448 C GLU 207 18.938 9.942 59.364 1.000 20.58 ANISOU 1448 C GLU 207 18.938 9.942 59.364 1.000 20.58 ANISOU 1448 C GLU 207 18.938 9.942 59.364 1.000 18.75 ATOM 1448 C GLU 207 18.938 9.942 59.364 1.000 20.58 ANISOU 1449 O GLU 207 18.938 1938 3684 -164 490 - 10 ATOM 1449 O GLU 207 18.8938 9.942 59.364 1.000 18.75 ATOM 1449 O GLU 207 18.665 8.612 30.449 52.8 -45 ATOM 1449 O GLU 207 18.665 8.612 30.449 52.8 -45 ATOM 1449 O GLU 207 18.665 8.612 30.449 52.8 -45 ATOM 1445 CG GLU 207 18.899 1794 4724 -19 83 -135 ATOM 1450 CB GLU 207 18.899 1794 4724 -19 83 -135 ATOM 1451 CG GLU 207 18.899 1794 4724 -19 83 -135 ATOM 1451 CG GLU 207 19.879 7.737 58.429 1.000 30.08 ANISOU 1451 CG GLU 207 19.879 7.737 58.429 1.000 29.99 3 ANISOU 1455 CD GLU 207 19.429 6.356 57.959 1.000 29.99 3 ANISOU 1455 CD GLU 207 5549 2024 3798 1179 -2099 -123 1452 CD GLU 207 19.429 6.356 57.959 1.000 29.93 ANISOU 1452 CD GLU 207 5549 2024 3798 ANISOU 1452 CD GLU 207 5549 2024 3798 1179 -2099 -123 ATOM 1453 OE1 GLU 207 19.491 5.471 58.839 1.000 35.14 ANISOU 1453 OE1 GLU 207 5782 2692 4879 938 -931 8 8 5 ATOM 1454 OE2 GLU 207 19.037 6.251 56.762 1.000 38.62 -ANISOU 1454 OE2 GLU 207 4955 5608 4109 135 -2494 -366 ATOM 1455 N VAL 208 21.146 10.997 59.414 1.000 16.97 ANISOU 1455 N VAL 208 1926 1974 2549 120 337 8 0 7 ATOM 1456 CA VAL 208 22.376 11.593 58.902 1.000 17.77 ANISOU 1456 CA VAL 208 22.376 11.593 58.902 1.000 17.77 ANISOU 1456 CA VAL 208 1894 2109 2748 93 500 4 1 1 ATOM 1457 CB VAL 208 22.455 13.111 59.155 1.000 16.89 ANISOU 1457 CB VAL 208 2774 2148 1494 -372 -149 5 6 9 ATOM 1458 CG1 VAL 208 23.652 13.688 58.409 1.000 20.76 ANISOU 1458 CG1 VAL 208 3214 2150 2526 -423 647 1 4 8 ATOM 1459 CG2 VAL 208 21.172 13.815 58.720 1.000 16.36 ANISOU 1459 CG2 VAL 208 3146 1640 1431 25 98 3 5 3 1179 -2099 - 123 ANISOU 1459 CG2 VAL 208 3146 1640 1431 25 98 3 5 3 ATOM 1460 C VAL 208 23.585 10.877 59.507 1.000 20.29 VAL 208 1936 2555 3217 11 -58 1 3 2 VAL 208 23.726 10.829 60.741 1.000 20.74 VAL 208 2436 2256 3187 460 206 5 4 GLY 209 24.457 10.295 58.672 1.000 18.94 GLY 209 1764 2445 2989 211 -494 1 ANISOU 1460 C 1461 0 MOTA ANISOU 1461 O 460 206 544 ATOM 1462 N ANISOU 1462 N 209 1764 2445 2989 211 -494 1 209 25.558 9.508 59.194 1.000 24.01 GLY-494 1 5 ATOM 1463 CA GLY ANISOU 1463 CA GLY GLY 209 2171 3040 3910 549 -396 7 0 GLY 209 25.123 8.364 60.082 1.000 25.00 GLY 209 2874 3156 3470 1406 772 64 549 -396 7 0 9 1464 C ATOM

1406 772 649

ANISOU 1464 C

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- 138 -
                      GLY 209 25.850 7.934 60.991 1.000 35.98 GLY 209 4448 3946 5279 1425 -426 1 GLY 210 23.951 7.786 59.869 1.000 25.89
          1465 0
 ANISOU 1465 0
                                                                    1425 -426 1769
          1466 N
                       GLY 210 3802
 ANISOU 1466 N
                                               2756
                             210 3802 2756
210 23.477 6.678
                                                         3278
                                                                    523
                                                                            899 749
ATOM
          1467 CA
                       GLY
                                                         60.671 1.000 26.43
ANISOU 1467 CA
                       GLY
                             210 4479
                                               2136
                                                         3427
                                                                    1228 742 912
          1468 C
ATOM
                             210 22.885 7.025
                       GLY
                                                         62.016 1.000 28.45
ANISOU 1468 C
                       GLY
                             210 5472 2099
                                                         3237
                                                                    831
                                                                            1029 1175
                             210 22 634 6.098 62.789 1.000 40.26
ATOM
          1469 0
                      GLY
                      GLY 210 7322 .2719 5256 1881 2759 2
ALA 211 22.651 8.281 62.338 1.000 25.78
ANISOU 1469 O
                                                                    1881 2759 2360
          1470 N
         1470 N ALA 211 4671 2359 2763 1370 724 1197
1471 CA ALA 211 22.048 8.671 63.613 1.000 23.74
1471 CA ALA 211 2966 3156 2896 727 339 663
1472 CB ALA 211 23.093 9.333 64.496 1.000 29.57
1473 C ALA 211 20.900 9.626 63.360 1.000 21.19
1474 O ALA 211 3090 2611 2350 484 178 741
1474 O ALA 211 3090 2659 2653 20.666 9
ANISOU 1470 N
                      ALA 211 4671 2359
ATOM
ANISOU 1471 CA
ATOM
ANISOU 1472 CB ALA
ANISOU 1473 C
ATOM
ANISOU 1474 O ALA
                             211 3771
                                              2659
                                                         2653
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                                                                          -66 930
ATOM
         1475 N
                      PHE
                             212 19.889 9.629
                                                         64.204 1.000 19.88
ANISOU 1475 N
                      PHE
                            212 2603
                                              2577
                                                        2375
                                                                    398
                                                                            -128 3 7 4
          1476 CA
                     PHE
                            212 18.814 10.613 64.130 1.000 19.13
ANISOU 1476 CA PHE
                            212 2581
                                              2257
                                                         2432
                                                                    284 -565 3 1 7
          1477 C
ATOM
                      PHE
                             212 19.320 12.006 64.489 1.000 20.00
ANISOU 1477 C
ANISOU 1477 C PHE 212 3004 2480 2115 133 -640 6 8 ATOM 1478 O PHE 212 19.893 12.230 65.569 1.000 21.10 ANISOU 1478 O PHE 212 2497 3558 1964 -391 -406 2 2 2 ATOM 1479 CB PHE 212 17.688 10.290 65.096 1.000 21.37 ANISOU 1479 CB PHE 212 2553 2616 2952 293 -197 - 1 8 4 ATOM 1480 CG PHE 212 17.010 8.950 64.912 1.000 23.45 ANISOU 1480 CG PHE 212 2161 3496 3253 -376 -282 -5 5 8 ATOM 1481 CD1 PHE 212 2161 3496 3253 -376 -282 -5 5 8 ATOM 1481 CD1 PHE 212 16.369 8.377 65.990 1.000 23.33 ANISOU 1481 CD1 PHE 212 2545 3115 3206 -382 -350 -5 0 8 ATOM 1482 CD2 PHE 212 17.029 8.302 63.687 1.000 25.83 ANISOU 1482 CD2 PHE 212 2554 3962 3299 -622 -217 -7 8 7
                      PHE
                             212 3004 2480
                                                         2115
                                                                    133 -640 6 8
ANISOU 1482 CD2 PHE
                            212 2554 · 3962
                                                        3299
                                                                   -622 -217 -787
                            212 15.730 7.149 65.872 1.000 28.13
ATOM
          1483 CE1 PHE
ANISOU 1483 CE1 PHE
                            212 3784 3544 3362
                                                                    -1119 96 - 973
                            212 16.419 7.072 63.569 1.000 23.04
212 2504 2960 3289 382 -232 -5
212 15.781 6.486 64.651 1.000 27.88
212 3658 3977 2957 -1072 -501 -7
213 19.076 12.936 63.578 1.000 18.30
213 2690 2083 2181 149 -583 -9
         1484 CE2 PHE
ATOM
ANISOU 1484 CE2 PHE
                                                                    382 -232 - 558
         1485 CZ PHE
ANISOU 1485 CZ
                     PHE
                                                                   =1072 -501 - 760
ATOM
         1486 N
                      THR
ANISOU 1486 N
                            213 2690
                      THR
                                              2083
                                                         2181
                                                                    149 -583 - 93
                            213 19.566 14.310 63.681 1.000 17.99
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         1487 CA THR
ANISOU 1487 CA THR
                            213 1976
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         1488 CB THR
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ANISOU 1488 CB THR
                            213 1798
                                              2280
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ANISOU 1489 OG1 THR
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                                                                    925 71 5 2 8
         1490 CG2 THR
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ANISOU 1490 CG2 THR
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                                                                    -310 -289 - 747
         1491 C
                             213 18.391 15.277 63.641 1.000 15.53
                      THR
ANISOU 1491 C
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213 17.533 15.195 62.761 1.000 16.11
213 1742 2197 2180 -327 -669 5
                      THR
                                                                          -557 - 167
ATOM
          1492 0
                      THR
ANISOU 1492 O
                      THR
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                             214 18.362 16.199 64.590 1.000 15.60
ATOM
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                      ASP
ANISOU 1493 N
                      ASP
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                                              2046
                                                                    64 - 405 2
                             214 17.380 17.256 64.672 1.000 15.59
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ANISOU 1494 CA
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         1495 CB
                             214 17.744 18.200 65.822 1.000 17.13
                      ASP
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- 139 -
 ANISOU 1495 CB ASP 214 2528
                                                                      1893
                                                                                      2086
                                                                                                      -226 -1022 -247
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 ANISOU 1496 CG ASP
                                           214 3138
                                                                      2495
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                                                                                                       -451 -1276 -148
               1497 OD1 ASP 214 17.079 16.571 67.460 1.000 20.87
 ANISOU 1497 OD1 ASP
                                           214 2778 2632
                                                                                      2518
                                                                                                      -247 -505 1 5 1
             1498 OD2 ASP
                                           214 18.076 18.401 68.127 1.000 28.05
 ANISOU 1498 OD2 ASP
                                           214 5110 3118
                                                                                      2429
                                                                                                      -257 -1997 -619
             1499 C ASP
 ATOM
                                           214 17.314 18.146 63.441 1.000 15.14
 ANISOU 1499 C
                                  ASP
                                           214 2029 1822 1901
                                                                                                    182 -574 - 319
                               ASP 214 18.349 18.552 62.897 1.000 17.63
 MOTA
                1500 O
 ANISOU 1500 O
                                           214 1956 2032 2710 -214 -810 - 15
215 16.105 18.493 63.027 1.000 14.69
                                 ASP
               1501 N
 ATOM
                                  LEU
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 ANISOU 1501 N
 ATOM
 ANISOU 1502 CA LEU
 MOTA
 ANISOU 1503 CB LEU 215 1735 2167 1506 -98 75 - 3
ATOM 1504 CG LEU 215 16.291 17.813 60.056 1.000 16.39
 ANISOU 1504 CG LEU 215 2031 2285 1911 -340 320 -4
ATOM 1505 CD1 LEU 215 15.517 16.999 59.031 1.000 22.61
                                                                                                      -340 320 -424
ATOM 1505 CD1 LEU 215 15.517 16.999 59.031 1.000 22.61 ANISOU 1505 CD1 LEU 215 3139 2024 3427 -10 -801 -87 ATOM 1506 CD2 LEU 215 17.482 18.543 59.434 1.000 26.93 ANISOU 1506 CD2 LEU 215 1998 5409 2827 -1083 909 -54 ATOM 1507 C LEU 215 15.002 20.622 62.500 1.000 14.65 ANISOU 1507 C LEU 215 1770 1607 2190 86 -165 -95 ATOM 1508 O LEU 215 13.822 20.662 62.151 1.000 19.45 ANISOU 1508 O LEU 215 1748 2165 3476 116 -303 -20 ATOM 1509 N PRO 216 15.552 21.523 63.314 1.000 15.99 ANISOU 1509 N PRO 216 2390 1970 1715 -164 21 -175 ATOM 1510 CD PRO 216 16.955 21.601 63.757 1.000 19.37 ANISOU 1510 CD PRO 216 2900 2306 2155 83 -790 -54 ATOM 1511 CA PRO 216 14.760 22.620 63.846 1.000 18.68
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                                                                                                      -1083 909 - 542
                                                                                                                -303 - 203
               1510 CD PRO 216 2900 2306 2155 =83 -790 - 1511 CA PRO 216 14.760 22.620 63.846 1.000 18.68
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 ATOM
 ANISOU 1511 CA PRO 216 3104
                                                                      2017
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              1512 CB PRO 216 15.649 23.227 64.949 1.000 18.63
ATOM 1512 CB PRO 216 15.649 23.227 64.949 1.000 18.63

ANISOU 1512 CB PRO 216 3592 1517 1971 -120 -421 9

ATOM 1513 CG PRO 216 17.030 22.847 64.581 1.000 22.35

ANISOU 1513 CG PRO 216 3401 2426 2666 -419 -427 - 78

ATOM 1514 C PRO 216 14.461 23.700 62.819 1.000 18.50

ANISOU 1514 C PRO 216 2921 2083 2026 58 -465 -473

ATOM 1515 O PRO 216 15.024 23.854 61.731 1.000 19.82

ANISOU 1515 O PRO 216 2752 2453 2325 -32 -375 1 9

ATOM 1516 N TYR 217 13.487 24.536 63.194 1.000 20.05

ANISOU 1516 N TYR 217 3213 1981 2422 90 -482 -718

ATOM 1517 CA TYR 217 13.178 25.662 62.308 1.000 22.97

ANISOU 1518 C TYR 217 14.347 26.647 62.283 1.000 23.92

ANISOU 1518 C TYR 217 4139 2131 2819 -337 -1776 -1
ATOM
                                                                                                      -419 -427 - 783
                                                                                                      211 -1467 -313
 ANISOU 1518 C
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TYR 217 15.149 26.726 63.213 1.000 30.46
                                                                                                      -337 -1776 -165
 MOTA
               1519 0
ANISOU 1519 O TYR 217 15.149 26.726 63.213 1.000 30.46

ANISOU 1519 O TYR 217 4321 3440 3812 -1118 -2477 7

ATOM 1520 CB TYR 217 11.891 26.314 62.768 1.000 32.68

ANISOU 1520 CB TYR 217 3958 3294 5164 1148 -874 -7

ATOM 1521 CG TYR 217 12.064 27.462 63.718 1.000 44.77

ANISOU 1521 CG TYR 217 6829 4326 5854 895 38 -187

ATOM 1522 CD1 TYR 217 11.853 28.763 63.285 1.000 54.26

ANISOU 1522 CD1 TYR 217 10311 3688 6615 -323 132 -1

ATOM 1523 CD2 TYR 217 10635 5155 6158 -1027 -1446 -
 ANISOU 1519 O
                                                                                                      -1118 -2477 728
                                                                                                      1148 -874 - 783
                                                                                                                 38 - 1870
                                                                                                      -323 132 -1945
                                            217 10635 5155 6158 -102/-1440
217 12.011 29.816 64.174 1.000 60.33
 ANISOU 1523 CD2 TYR
                                                                                                      -1027 -1446 -1931
               1524 CE1 TYR
 ANISOU 1524 CE1 TYR
                                           217 11807
                                                                      4345
                                                                                      6772
                                                                                                      -1101 -132 -2259
                                           217 12.585 28.296 65.926 1.000 64.51
217 12481 5199 6832 -1936 -1520 -
               1525 CE2 TYR
 ANISOU 1525 CE2 TYR
                                                                                                      -1936 - 1520 - 2074
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- 140 -1526 CZ TYR 217 12.378 29.586 65.481 1.000 64.11 ATOM ATOM 1526 CZ TYR 217 12047 5183 7129 -1460 -817 -2160 ATOM 1527 OH TYR 217 12.536 30.639 66.358 1.000 63.69 ANISOU 1527 OH TYR 217 11840 5206 7153 218 14.418 27.374 61.188 1.000 24.08 -1832 -1191 -2064 ATOM 1528 N ARG ANISOU 1528 N 218 4482 ARG 1611 3055 218 15.335 28.465 60.948 1.000 30.71 -1471 - 145 ATOM 1529 CA ARG ANISOU 1529 CA ARG 218 5932 2490 3245 -504 -1565 382 218 16.326 28.135 59.840 1.000 35.08 ATOM 1530 CB ARG ANISOU 1530 CB ARG 218 5969 2797 4562 -1397 -779 - 348 1531 CG 218 17.401 27.114 60.073 1.000 35.77 ATOM ARG ANISOU 1531 CG ARG 218 6009 3087 4497 -1107 -733 - 773 1532 CD 218 18.658 27.775 60.626 1.000 34.46 ARG ANISOU 1532 CD 218 5680 3264 4152 -1242 -244 - 6 218 19.223 28.746 59.709 1.000 29.51 ARG -1242 -244 - 619 1533 NE ARG ANISOU 1533 NE ARG 218 4707 2579 3926 78 81 -629 218 20.218 28.620 58.830 1.000 33.18 MOTA 1534 CZ ARG ANISOU 1534 CZ ARG 218 5269 3166 4170 60 452 -1075 218 20.839 27.452 58.709 1.000 27.44 1535 NH1 ARG ANISOU 1535 NH1 ARG 218 4202 2881 3341 -503 -373 -1585 1536 NH2 ARG 218 20.583 29.675 58.077 1.000 22.96 ATOM ANISOU 1536 NH2 ARG 218 2327 3579 2817 23,3 -1117 -872 ATOM 1537 C ARG 218 14.513 29.655 60.464 1.000 31.05 ANISOU 1537 C ARG 218 7353 1949 2496 -448 -1823 197 ATOM 1538 0 218 14.114 29.533 59.295 1.000 40.40 ARG ANISOU 1538 O 218 9873 2241 3235 531 -3168 -219 14.246 30.747 61.157 1.000 30.01 ARG -3168 - 627 ATOM 1539 N PRO 1539 N PRO 219 6290 2559 2555 -499 -1839 -1540 CD PRO 219 14.597 31.043 62.543 1.000 36.79 ANISOU 1539 N -499 -1839 -284 - ATOM ANISOU 1540 CD PRO 219 8147 2878 2954 -1848 -2548 ATOM 1541 CA PRO 219 13.464 31.841 60.549 1.000 26.34 -1848 -2548 - 374 ANISOU 1541 CA PRO 219 4421 1541 CA PRO 219 4421 2564 3025 -573 -988 - 3
1542 CB PRO 219 13.523 32.993 61.563 1.000 32.44
1543 CG PRO 219 5361 2891 4073 -691 -417 - 9
1543 CG PRO 219 13.947 32.372 62.825 1.000 38.75
1544 C PRO 219 14.005 32.329 59.220 1.000 23.64
1545 O PRO 219 3472 2066 3443 -161 -1028 1
1545 O PRO 219 13.300 32.950 58.412 1.000 30.61
1546 N ASP 220 15 260 3344 43 -347 -1712 8 256.4 3025 -573 -988 - 340 ATOM ANISOU 1542 CB -691 -417 - 989 ATOM ANISOU 1543 CG -1981 -958 -1235 ANISOU 1544 C -161 -1028 1 0 9 ATOM ANISOU 1545 O PRO -347 -1712 8 7 6 1546 N ASP ATOM ANISOU 1546 N ASP 220 3611 1756 1547 CA ASP 220 15.847 32.660 57.705 1.000 27.96 4506 -389 -644 -815 ATOM ANISOU 1547 CA ASP 220 3951 1603 5071 -364 30 - 824 ATOM ASP 220 17.212 33.238 58.155 1.000 29.61 1548 CB ANISOU 1548 CB ASP 220 3549 3142 4558 -176 -326 1 7 6 ASP 220 18.091 32.158 58.780 1.000 32.09 ASP 220 3706 3527 4961 625 978 61 ASP 220 17.697 31.434 59.719 1.000 26.12 ASP 220 3013 3522 3390 -158 -289 -2 ATOM 1549 CG ANISOU 1549 CG 625 978 615 1550 OD1 ASP ANISOU 1550 OD1 ASP 220 3013 3522 3390 -158 -289 -220 19.241 32.088 58.281 1.000 29.09 220 3714 3756 3581 304 677 --158 - 289 - 97ATOM 1551 OD2 ASP ANISOU 1551 OD2 ASP 677 - 712 ASP 220 16.037 31.726 56.525 1.000 25.26 ATOM 1552 C 1552 C ASP 220 2508 1291 5800 354 1110 - 8 1553 O ASP 220 16.641 32.095 55.515 1.000 28.28 ANISOU 1552 C 354 1110 - 822 ATOM ANISOU 1553 O ASP 220 4088 ASP 220 4088 1665 4994 -855 298 -4 ALA 221 15.500 30.510 56.631 1.000 21.58 -855 298 -434 ATOM 1554 N ANISOU 1554 N ALA 221 2748 ALA 221 15.840 29.484 55.658 1.000 19.81 1770 -288 178 -651 ATOM 1555 CA ANISOU 1555 CA 221 2986 1452 ALA3090 -342 -224 -315221 17.130 28.800 56.109 1.000 19.51 ATOM 1556 CB ALA

- 141 -ANISOU 1556 CB ALA 221 2267 1497 3647 -648 45 -74 ATOM 1557 C ALA 221 14.718 28.469 55.489 1.000 17.71 ANISOU 1557 C ALA 221 2304 1912 2512 -251 -75 -3 ATOM 1558 O ALA 221 13.866 28.356 56.380 1.000 20.97 3647 -648 45 - 746 -251 -75 -309 ANISOU 1558 O ALA 221 3596 2029 2344 ~503 406 -284 1559 N VAL 222 14.728 27.756 54.378 1.000 14.22 ANISOU 1559 N VAL 222 1560 1582 2262 -76 -92 -11 ATOM 1560 CA VAL 222 13.823 26.617 54.160 1.000 14.89 ANISOU 1560 CA VAL 222 1326 1608 2723 98-216 -205 ATOM 1561 CB VAL 222 13.079 26.779 52.830 1.000 17.28 ANISOU 1561 CB VAL 222 1680 175 4 3133 90-657 -144 ANISOU 1561 CB VAL 222 1680 1754 3133 90 -657 -144
ATOM 1562 CG1 VAL 222 13.995 26.685 51.620 1.000 19.17
ANISOU 1562 CG1 VAL 222 1974 2625 2686 -446 -775 150
ATOM 1563 CG2 VAL 222 11.996 25.747 52.641 1.000 17.36
ANISOU 1563 CG2 VAL 222 2185 1879 2533 -254 -362 -385
ATOM 1564 C VAL 222 14.653 25.339 54.263 1.000 12.66
ANISOU 1564 C VAL 222 1136 1564 2112 -50 -225 -378
ATOM 1565 O VAL 222 15.828 25.320 53.893 1.000 13.12
ANISOU 1566 N LEU 223 14.049 24.267 54.775 1.000 12.98
ANISOU 1566 N LEU 223 14.681 22.952 54.749 1.000 10.70
ANISOU 1567 CA LEU 223 891 1704 1472 -26 -98 - 7 ATOM 1567 CA LEU 223 14.681 22.952 54.749 1.000 10.70 ANISOU 1567 CA LEU 223 891 1704 1472 -26 -98 - 7 ATOM 1568 CB LEU 223 14.276 22.130 55.961 1.000 13.02 ANISOU 1568 CB LEU 223 1387 1968 1593 -419 289 -1 ATOM 1569 CG LEU 223 14.739 20.683 56.106 1.000 17.41 ANISOU 1569 CG LEU 223 2434 2132 2050 -290 -476 56 ATOM 1570 CD1 LEU 223 16.247 20.614 56.204 1.000 17.20 ANISOU 1570 CD1 LEU 223 2576 1518 2441 26 -989 -24 ATOM 1571 CD2 LEU 223 13.983 20.076 57.282 1.000 33.63 ANISOU 1571 CD2 LEU 223 3981 4721 4077 -341 134 29 ATOM 1572 C LEU 223 14.362 22 211 53.456 1.000 10.02 -419 289 -108 -290 -476 5 6 6 26 - 989 - 249 ANISOU 1571 CD2 LEU 223 3981 4721 4077 -341 134 294 ATOM 1572 C LEU 223 14.362 22.211 53.456 1.000 10.02 ANISOU 1572 C LEU 223 1000 1265 1543 58 -319 8 8 ATOM 1573 O LEU 223 13.206 22.160 53.088 1.000 12.86 ANISOU 1573 O LEU 223 949 1945 1992 -97 -174 -372 4077 -341 134 2949 ATOM 1573 O LEU 223 13.206 22.160 53.088 1.000 12.86
ANISOU 1573 O LEU 223 949 1945 1992 -97 -174 -372
ATOM 1574 N VAL 224 15.406 21.675 52.798 1.000 10.55
ANISOU 1574 N VAL 224 978 1070 1962 -76 -418 -382
ATOM 1575 CA VAL 224 15.227 20.932 51.553 1.000 11.98
ANISOU 1575 CA VAL 224 1376 1288 1887 -249 -278 -372
ATOM 1576 CB VAL 224 16.095 21.461 50.391 1.000 11.23
ANISOU 1576 CB VAL 224 16.095 21.461 50.391 1.000 11.23
ANISOU 1577 CG1 VAL 224 15.833 20.690 49.102 1.000 13.16
ANISOU 1577 CG1 VAL 224 1899 1485 1615 -462 -516 8 4
ATOM 1578 CG2 VAL 224 1480 1520 2266 -135 -354 -6 4
ATOM 1578 CG2 VAL 224 15.539 19.450 51.786 1.000 10.87
ANISOU 1579 C VAL 224 15.539 19.450 51.786 1.000 10.87
ANISOU 1579 C VAL 224 16.646 19.148 52.201 1.000 12.57
ANISOU 1580 O VAL 224 1283 1363 2132 -175 -154 -2 7 4
ATOM 1580 O VAL 224 1283 1363 2132 -175 -154 -2 7 4
ATOM 1581 N PHE 225 14.585 18.553 51.533 1.000 11.86
ANISOU 1582 CA PHE 225 14.811 17.130 51.412 1.000 11.38
ANISOU 1582 CA PHE 225 1241 1128 2137 -15 -303 -6 1
ATOM 1583 CB PHE 225 1260 1157 1909 -22 -67 -56
ATOM 1583 CB PHE 225 13.707 16.280 52.044 1.000 11.38
ANISOU 1583 CB PHE 225 13.654 16.172 53.544 1.000 11.38
ANISOU 1583 CB PHE 225 13.654 16.172 53.544 1.000 11.38
ANISOU 1583 CB PHE 225 13.654 16.172 53.544 1.000 11.38
ANISOU 1585 CD1 PHE 225 14.685 15.653 54.251 1.000 15.28
ANISOU 1586 CD2 PHE 225 12.532 16.576 54.254 1.000 17.91
ANISOU 1586 CD2 PHE 225 12.532 16.576 54.254 1.000 17.991
ANISOU 1586 CD2 PHE 225 12.532 16.576 54.254 1.000 17.991
ANISOU 1586 CD2 PHE 225 12.532 16.576 54.254 1.000 17.991
ANISOU 1586 CD2 PHE 225 12.532 16.576 54.254 1.000 17.991

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- 142 -
         1587 CE1 PHE 225 14.619 15.535 55.661 1.000 17.46
ANISOU 1587 CE1 PHE 225 2449
                                       1862
                                                 2321
                                                           -249 -795 6 6 6
         1588 CE2 PHE 225 12.447 16.474 55.612 1.000 19.35 1588 CE2 PHE 225 2563 2678 2111 121 129 -
ANISOU 1588 CE2 PHE
                                                           121 129 - 11
         1589 CZ
ATOM
                   PHE
                        225 13.499 15.945 56.341 1.000 18.20
                        225 2952 1641 2324 -501 -470 3
225 14.907 16.774 49.927 1.000 12.03
225 1480 1285 1804 130 -201 4
225 14.019 17.160 49.163 1.000 12.77
ANISOU 1589 CZ
                   PHE
                                                          -501 -470 3 6
ATOM
        1590 C
                   PHE
ANISOU 1590 C
                   PHE
                                                                -201 4 2
ATOM
        1591 0
                   PHE
                        ANISOU 1591 O
                   PHE
                                                          341 -118 3 8
        15.92 N
                   CYS
                        226 954 1403 1296
ANISOU 1592 N
                   CYS
                                                    -204 -407
ATOM
        1593 CA CYS
                        226 15.917 15.400 48.197 1.000 10.80
ANISOU 1593 CA CYS 226 1432
                                       1204
        1594 CB CYS 226 17.337 15.029 47.744 1.000 12.02
                                                 1468
                                                          -258 -310 - 59
ATOM
ANISOU 1594 CB
                  CYS 226 1539
                                       1362
                                                 1666
                                                          -357
                                                                16 - 125
        1595 SG
                  CYS 226 18.426 16.4' 0 47.554 1.000 13.74
CYS 225 1627 1400 2192 -341 18 13 9
ANISOU 1595 SG
ATOM 1596 C
                   CYS 226 14.998 14.178 48.256 1.000 9.86

CYS 226 1190 1061 1495 -20 -293 - 1000 11.17

CYS 226 15.015 13.431 49.252 1.000 11.17

CYS 226 1181 1280 1781 -129 -435 25

GLY 227 14.217 13.963 47.205 1.000 10.17

GLY 227 1428 1010 1427 -258 -271 - 3
                                                                 18 1 3 9
ANISOU 1596 C
                                                               -293 - 16
ATOM
        1597 0
ANISOU 1597 O
                                                          -129 -435 2 7 2
ATOM
        1598 N
ANISOU 1598 N
                        ATOM
        1599 CA GLY
ANISOU 1599 CA GLY
                        227 1231 860 1604
                        227 13.908 11.769 46.074 1.000 9.48
227 1438 717 1445 1-6 -35 169
                                                     -178 -74 - 37
ATOM
        1600 C
                  GLY
ANISOU 1600 C
                        227 1438
                   GLY
                  GLY 227 14.935 11.961 45.402 1.000 9.86
ATOM
        1601 0
                  GLY 227 1321 1137 1290 -104 -179 7

ALA 228 13.217 10.631 45.971 1.000 9.17

ALA 228 1279 729 1477 1.09 -135 5 8

ALA 228 13.650 9.529 45.108 1.000 9.41

ALA 228 1315 887 1371 9 -74 -52

ALA 228 12.727 8.296 45.256 1.000 10.50
ANISOU 1601 O
                                                          -104 -179 7 8
ATOM
        1602 N
ANISOU 1602 N
ATOM
        1603 CA
ANISOU 1603 CA
        1604 CB
ANISOU 1604 CB ALA 228 2011
                                       824 1155 -143 124 1 0 1
                  ALA 228 13.712 9.918 43.637 1.000 9.25
ATOM
        1605 C
ANISOU 1605 C
                   ALA 228 1343
                                       666 1507 -108 90 1 3 9
        1606 0
                  ALA 228 14.493 9.305 42.895 1.000 9.48
ATOM
ANISOU 1606 O
                   ALA 228 1171
                                       1026
                                                1405
                                                          -88
                                                                 -50 9 0
ATOM
        1607 N
                   ILE 229 12.970 10.907 43.143 1.000 10.30
ANISOU 1607 N
                        229 1402 1004 1509 18 25 1 7 7
229 13.074 11.311 41.727 1.000 10.87
229 1197 1446 1487 -2 -159 25 1
229 11.802 12.078 41.295 1.000 11.52
                   ILE
ATOM
        1608 CA
                   ILE
ANISOU 1608 CA
                   ILE
                                                          -2 -159 251
ATOM
        1609 CB
                   ILE
ANISOU 1609 CB
                   ILE
                         229 1257 1473 1647 34 -57 3 6 2
229 11.997 12.852 39.999 1.000 11.30
ATOM
        1610 CG2 ILE
ANISOU 1610 CG2 ILE
                        229 1655 1211 1426 83 -189 150
229 10.575 11.131 41.237 1.000 14.39
                                                          83 - 189 156
        1611 CG1 ILE
MOTA
ANISOU 1611 CG1 ILE
                        229 1031
                        229 1031 2034 2402 -40 210 3
229 10.676 10.093 40.138 1.000 19.20
                                                                210 311
ATOM
        1612 CD1 ILE
ANISOU 1612 CD1 ILE
                        229 2085
                        229 2085 1723 3489 -610 93 -138
229 14.389 12.034 41.477 1.000 10.38
        1613 C
                   ILE
ANISOU 1613 C
                   ILE
                        229 1293
                                                                 -169 3 2 2
ATOM
        1614 0
                   ILE
ANISOU 1614 O
                   ILE 229 1805
                                       1257
                                                1368
                                                          -13
                                                               145 3 2 8
MOTA
        1615 N
                   ALA 230 14.965 12.692 42.490 1.000 10.66
ANISOU 1615 N
                   ALA
                        230 1476
                                       1274
                                                1300 -104 -151 3 5 6
                        230 16.312 13.259 42.338 1.000 11.21
        1616 CA
                  ALA
ANISOU 1616 CA
                   ALA
                         230 1473
                                       975 1813
                                                     -57 -308 9 0
        1617 CB
                   ALA
                         230 16.681 14.148 43.509 1.000 10.58
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						- 143 -		
ANISOU	1617	СВ	ALA	230	1350	1295	1375	62 - 106 126
ATOM	1618	С	ALA	230	17.336	12.136	42.132	1.000 11.28
ANISOU	1618	С	ALA	230	1640	1037	1610	1 55 2 4 2
ATOM	1619	0	ALA	230	18.220	12.185	41.273	1.000 11.29
ANISOU	1619	О	ALA	230	1510	1240	1539	-189 -40 288
ATOM	1620	N	THR	231	17.173	11.097		1.000 10.55
ANISOU	1620	Ν	THR		1328	894 17		
ATOM	1621		THR	231	18.064	9.939	42.819	1.000 11.98
ANISOU	1621	CA	THR		1929	1018	1605	0 -164 159
ATOM	1622	СВ	THR	231	17.717	8.865	43.878	1.000 10 . 76
ANISOU			THR	231	1381	1070	1636	-86 -453 2 4 6
ATOM	1623			231	17.658	9.437	45.198	1.000 11.82
ANISOU	1623	OG1	THR	231	1615	1236	1641	35 -115 277
ATOM	1624			231	18.765	7.752	43.880	1.000 12.57
ANISOU					1621	1314	1840	160 -89 351
ATOM	1625		THR		17.958	9.352	41.415	1.000 12.52
ANISOU			THR	231	1632	1500	1624	-145 42 1 1
ATOM	1626		TI.R		18.939	9.050	40.732	1.000 12.15
ANISOU			THR		1636	1233	1747	-17 86 2 2 4
ATOM	1627		LEU		16.717	9.154	40.959	1.000 11.14
ANISOU			LEU		1608	1005	1620	90 -68 1 4 1
ATOM	1628		LEU		16.446	8.522	39.675	1.000 12.47
ANISOU			LEU		1880	1203	1657	109 -169 4 5
ATOM	1629		LEU	232	14.950	8.214	39.552	1.000 12.81
ANISOU			LEU		1989	1225	1654	-78 -209 1 9
ATOM ANISOU	1630	CG	LEU		14.452	7.464	38.314	1.000 14:85
ANISOU	1631		LEU		2171	1753	1719	-5 -410 - 96
ANISOU	1631	CDI	TEU	232	15.020 2693	6.055	38.240	1.000 16.78
-ATOM	1632	CD3	LEU		12.914	1749	1932	72 -431 -487
ANISOU	1632	CD2	LEU		2180	7.411 1866	38.291 1920	1.000 15.70 -278 -589 4 9 4
ATOM	1633		LEU		16.964	9.354	38.511	-278 -589 4 9 4 1.000 11.58
ANISOU			LEU		1452	1390	1559	309 -301 1 3 6
ATOM	1634		LEU	232	17.752	8.837	37.686	1.000 13.45
ANISOU			LEU		1808	1436	1867	320 -17 3 0
ATOM	1635		VAL	233		10.617	38.414	1.000 10.95
ANISOU			VAL		1428	1210	1522	-14 -210 0
ATOM	1636		VAL		16.948	11.421	37.242	1.000 11.70
ANISOU	1636	CA	VAL	233	1703	1345	1397	975 1 3
MOTA	1637		VAL	233	16.156	12.743	37.215	1.000 11.14
ANISOU			VAL		1672	1272	1287	-26 276 7 3
MOTA	1638	CG1	VAL		16.661	13.774	38.249	1.000 13.34
ANISOU	1638	CG1	VAL	233	1834	1562	1673	-205 653 -368
ATOM	1639	CG2	VAL		16.106	13.412	35.827	1.000 14.66
ANISOU					1992	1873	1704	-4 -45 5 8 6
ATOM	1640		VAL		18.459	11.586	37.132	1.000 13.41
ANISOU			VAL		1712	1573	1811	91 151 1 2 5
ATOM	1641		VAL		19.012	11.627	36.021	1.000 13.45
ANISOU ATOM	1642		VAL		1844	1402	1866	46 192 4 3 8
ANISOU			THR		19.188	11.665	38.250	1.000 13.13
ANISOU	1643	N C A	THR THR		1457	1639	1893	-139 223 126
ANISOU	1643	CA	THR		20.613	11.930		1.000 13.00
ATOM	1644		THR		1483 21.069	1600	1855	-188 428 143
ANISOU			THR		1300	12.726	39.465	1.000 12.46 -32 200 251
ATOM	1645	OG1			20.825	1632	1803	
ANISOU		OG1		234	1660	11.941 1662	40.639 1888	1.000 13.71 192 202 291
ATOM	1646				20.301	14.027	39.643	1.000 11.37
ANISOU	1646	CG2	THR		1097	1565	1657	-153 -87 169
ATOM	1647	C	THR		21.424	10.643	38.178	1.000 14.44
ANISOU			THR		1550	1823	2114	6 -73 - 5 3
				-		<del></del>		

- 144 -1648 0 THR 234 22.659 10.710 38.233 1.000 15.81 ANISOU 1648 O THR 234 1546 2169 2293 61 27 2 1 7 1649 N GLY 235 20.767 9.477 38.070 1.000 14.76 ANISOU 1649 N GLY 235 1776 1576 2254 77 81 410 1650 CA ATOM GLY 235 21.530 8.249 37.994 1.000 16.69 ANISOU 1650 CA 235 2053  $\operatorname{\mathsf{GL}} \operatorname{\mathsf{Y}}$ 1803 2486 304 35 1 8 9 1651 C ATOM 235 22.243 7.862 GLY39.275 1.000 16.83 ANISOU 1651 C GLY 235 1854 2031 2512 765 244 193 MOTA 1652 0 235 23.305 7.237 GLY 39.194 1.000 19.67 ANISOU 1652 O GLY 235 2074 2172 3225 1035 383 372 ATOM 1653 N GLY 236 21.665 8.227 40.425 1.000 14.46 236 1732 1327 2433 154 198 7 236 22.187 7.768 41.692 1.000 15.73 236 2060 1381 2536 41 186 3 1 2 236 23.166 8.691 42.388 1.000 14.76 236 1931 1332 2346 252 73 2 8 8 ANISOU 1653 N GLY 198 7 5 ATOM 1654 CA  ${ t GLY}$ ANISOU 1654 CA GLY1655 C GLY ANISOU 1655 C GLY 2346 252 73 2 8 8 ATOM 1656 C 236 23.778 8.244 GLY43.373 1.000 18.32 ANISOU 1656 O GLY 236 1983 2197 2782 106 -105 8 4 4 ATOM 1657 N 237 23.318 9.938 GLN 41.953 1.000 13.99 ANISOU 1657 N GLN237 1831 1349 2137 158 165 170 ATOM 1658 CA GLN237 24.209 10.956 42.485 1.000 13.13 ANISOU 1658 CA GLN 237 1474 1304 2210 367 -31 276 ATOM 1659 CB GLN 237 24.629 11.948 41.383 1.000 13.38 ANISOU 1659 CB GLN 237 1367 1566 2151 99 72 1 5 9 1660 CG GLN 237 25.390 11.335 40.219 1.000 14.74 237 1404 1529 2666 518 410 3 237 25.816 12.428 39.257 1.000 17.22 237 2039 2018 2486 -64 426 3 237 26.754 13.208 39.522 1.000 20.60 ANISOU 1660 CG GLN 518 410 333 ATOM 1661 CD GLN ANISOU 1661 CD GLN 426 360 ATOM 1662 OE1 GLN ANISOU 1662 OE1 GLN 237 1566 2334 3928 -10 -29 965 237 25.116 12.470 38.127 1.000 17.47 ATOM 1663 NE2 GLN ANISOU 1663 NE2 GLN 237 2014 2093 2533 208 438 408 237 23.627 11.739 43.663 1.000 12.90 ATOM 1664 C GLN ANISOU 1664 C GLN 237 1474 1324 2104 72 -10 2 5 5 ATOM 1665 0 237 24.332 12.549 44.282 1.000 15.90 GLN ANISOU 1665 O GLN 237 1739 1888 2413 -291 74 - 84 1666 N ATOM 238 22.365 11.481 44.013 1.000 12.13 VAL ANISOU 1666 N VAL ATOM 1667 CA VAL ANISOU 1667 CA VAL 238 1169 1436 1920 -121 -276 -19ATOM 238 20.622 13.158 44.510 1.000 12.00 1668 CB VAL ANISOU 1668 CB VAL 238 1024 1179 2357 -6 199 - 3 1 1669 CG1 VAL ATOM 238 19.978 13.999 45.601 1.000 13.07 ANISOU 1669 CG1 VAL 238 1530 1668 1767 63 -232 - 222 238 21.207 14.088 43.463 1.000 14.00 1670 CG2 VAL ANISOU 1670 CG2 VAL 238 1795 1470 2053 -40 -2 1 8 1 ATOM 238 20.990 11.156 46.000 1.000 13.62 1671 C VAL ANISOU 1671 C VAL 238 1707 1415 2054 -103 -40 - 22MOTA 1672 0 238 20.252 10.288 45.492 1.000 12.64 VAL ANISOU 1672 O 238 1702 VAL 977 2123 60 -318 257 ATOM 1673 N 239 21.247 11.246 47.300 1.000 11.99 239 1075 1404 2076 127 -1017 LYS ANISOU 1673 N LYS 1404 2076 127 -101 7 4 239 20.568 10.444 48.322 1.000 12.77 ATOM 1674 CA LYS ANISOU 1674 CA LYS 239 1224 1541 2088 -12 239 21.382 10.463 49.622 1.000 12.23 ATOM 1675 CB LYS ANISOU 1675 CB LYS 239 1333 1155 2158 183 -234 - 28 1676 CG 239 20.953 9.626 LYS 50.793 1.000 13.85 ANISOU 1676 CG LYS 239 1643 1689 1931 187 -52 -89 1677 CD ATOM LYS 239 21.927 9.579 51.957 1.000 20.13 ANISOU 1677 CD LYS 239 2893 1795 2961 10 -1185 5 8 8 1678 CE 239 21.364 8.745 53.098 1.000 24.73 ATOM LYS

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		- 145 -		
ANISOU 1678 CE	LYS 239 4		3080	-348 -1466 1064
ATOM 1679 NZ ANISOU 1679 NZ		2.019 8.841	54.420	
ATOM 1680 C	LYS 239 5 LYS 239 1		2293	1610 -930 - 304
ANISOU 1680 C	LYS 239 1 LYS 239 1		48.661	1.000 11.59
ATOM 1681 O	LYS 239 1	207 1332 8.976 12.191	1866	-35 -82 6 4
ANISOU 1681 O	LYS 239 1	638 1294	48.708 1749	1.000 12.32
ATOM 1682 N	ALA 240 1	8.222 10.047	48.863	-2 -25 2 3 6 1.000 10.65
ANISOU 1682 N	ALA 240 1	248 1266	1534	-52 <i>-</i> 185 <i>-</i> 88
ATOM 1683 CA	ALA 240 1		49.354	1.000 10.21
ANISOU 1683 CA	ALA 240 1	292 1057	1531	-195 -37 -109
ATOM 1684 CB	ALA 240 1	5.784 9.782		1.000 13.46
ANISOU 1684 CB	ALA 240 1		1543	-232 20 -403
ATOM 1685 C ANISOU 1685 C	ALA 240 1		50.807	1.000 10.97
ATOM 1686 O	ALA 240 1 ALA 240 1		1611	-127 -142 4 9
ANISOU 1686 O	ALA 240 1 ALA 240 2		51.059	1.000 13.02
ATOM 1687 N	PRO 241 1		1568 51.782	-243 28 - 7
ANISOU 1687 N	PRO 241 1			1.000 11.13 160 -49 138
ATOM 1688 CD	PRO 241 1			
ANISOU 1688 CD	PRO 241 1	419 1204		-180 -128 7 6
ATOM 1689 CA	PRO 241 1		53.166	1.000 11.96
ANISOU 1689 CA	PRO 241 1			-172 -32 193
ATOM 1690 CB ANISOU 1690 CB	PRO 241 11 PRO 241 11		53.891	1.000 14.25
ATOM 1691 CG	PRO 241 1: PRO 241 1:			-531 -383 2 4 2
ANISOU 1691 CG	PRO 241 2			1.000 13.61 -596 -465 - 22
ATOM 1692 C	PRO 241 1:			1.000 12.35
ANISOU 1692 C	PRO 241 1			-175 -187 4 1 8
ATOM 1693 O	PRO 241 1			1.000 12.28
ANISOU 1693 O ATOM 1694 N	PRO 241 1:			-232 -468 8 1
ATOM 1694 N ANISOU 1694 N	ARG 242 15 ARG 242 1		54.711	1.000 12.75
ATOM 1695 CA		775 1407 4.563 8.804	1664	-170 76 2 5 0
ANISOU 1695 CA	ARG 242 1:			1.000 10.76 -207 -281 2 1 1
ATOM 1696 CB	ARG 242 1	4.614 7.405		1.000 15.02
ANISOU 1696 CB	ARG 242 24	419 1368		-357 117 294
ATOM 1697 CG	ARG 242 1		55.230	1.000 17.85
ANISOU 1697 CG	ARG 242 3:		2135	9 -560 251
ATOM 1698 CD ANISOU 1698 CD	ARG 242 14			1.000 19.42
ATOM 1699 NE	ARG 242 3: ARG 242 1:			506 503 116
ANISOU 1699 NE	ARG 242 1:	5.667 4.552 225 2107		1.000 20.71 938 638 212
ATOM 1700 CZ	ARG 242 1			1.000 23.22
ANISOU 1700 CZ	ARG 242 3:			307 -544 5 8 9
ATOM 1701 NH1		5.285 2.567		1.000 24.46
ANISOU 1701 NH1 ATOM 1702 NH2				307 387 195
ATOM 1702 NH2 ANISOU 1702 NH2		7.416 3.184		1.000 25.41
ATOM 1703 C				819 -267 4 0 3
ANISOU 1703 C	ARG 242 14 ARG 242 1	4.477 9.834 571 1463		1.000 11.95
ATOM 1704 O	ARG 242 1			-248 -214 1 0 7 1.000 13.65
ANISOU 1704 O	ARG 242 1	708 1439		-322 -401 - 38
ATOM 1705 N	HIS 243 1:	3.252 10.085		1.000 11.60
ANISOU 1705 N		657 1410	1342	-311 -206 5
ATOM 1706 CA ANISOU 1706 CA	HIS 243 1:			1.000 11.49
ATOM 1707 CB		855 1571	938 -30	
ANISOU 1707 CB	HIS 243 1:	2.968 12.462		1.000 11.22
ATOM 1708 CG	HIS 243 1:		1453 56.341	-231 -221 3 9
ANISOU 1708 CG	HIS 243 1	937 1171	1378	1.000 11.80
			1310	-31 -200 / 3

- 146 -1709 CD2 HIS 243 10.885 13.236 56.181 1.000 11.15 ANISOU 1709 CD2 HIS 243 1990 1106 1142 35 - 344 141 1710 ND1 HIS ATOM 243 12.538 124345 55.086 1.000 12.29 ANISOU 1710 ND1 HIS 243 1670 1606 1395 -394 -91 8 MOTA 1711 CE1 HIS 243 11.599 12.653 54.209 1.000 12.59 ANISOU 1711 CE1 HIS 243 1686 1740 1357 -522 -202 - 253 1712 NE2 HIS ATOM 243 10.585 13.204 54.841 1.000 10.77 243 1612 1307 1172 -616 -268 -ANISOU 1712 NE2 HIS 1172 -616 -268 - 3 6 243 11.605 10.737 58.812 1.000 12.49 1713 C HIS ANISOU 1713 C 243 1869 HIS 1308 -321 -53 7 3 1570 243 10.807 9.949 MOTA 1714 0 HIS 58.271 1.000 12.26 ANISOU 1714 O HIS 243 1756 1404 1497 -188 -115 4 7 HIS 244 11.352 11.319 59.983 1.000 12.16 1715 N ATOM ANISOU 1715 N HIS 244 1464 1715 1442 -230 -112 - 3 2 1716 CA HIS 244 10.138 11.043 60.758 1.000 12.02 MOTA ANISOU 1716 CA HIS 244 1606 1809 1152 -599 -167 - 24 1717 CB 244 10.255 9.778 61.615 1.000 12.51 ATOM HIS ANISOU 1717 CB HIS 244 1655 1763 -19 101 - 47 1334 ATOM 1718 CG HIS 244 11.270 9.810 62.698 1.000 15.04 ANISOU 1718 CG HIS 244 2025 1723 1965 -178 -433 1 5 4 1719 CD2 HIS 244 11.276 10.380 63.923 1.000 18.19 ANISOU 1719 CD2 HIS 244 2946 2339 1627 36 - 732 297 MOTA 1720 ND1 HIS 244 12.504 9.203 62.662 1.000 19.30 ANISOU 1720 ND1 HIS 244 2303 2232 2800 229 -708 2 6 6 1721 CE1 HIS ATOM 244 13.226 9.387 244 2649 2734 63.731 1.000 22.48 ANISOU 1721 CE1 HIS 3159 11 -1206 6 5 0 ATOM 1722 NE2 HIS 244 12.476 10.120 64.531 1.000 22.33 ANISOU 1722 NE2 HIS 244 3088 2895 2500 -272 -1236 384 MOTA 1723 C 244 9.780 244 1897 HIS 12.246 61.613 1.000 13.47 ANISOU 1723 C HIS 1673 1549 -362 254 6 7 1724 0 ATOM HIS 244 10.603 13.165 61.798 1.000 13.48 ANISOU 1724 O 244 1800 245 8.551 HIS 1726 1595 -283 139 -161 ATOM 1725 N VAL 12.245 62.130 1.000 15.26 VAL 245 1852 ANISOU 1725 N 1964 1983 -417 232 - 55 1726 CA VAL 245 8.090 ATOM 13.352 62.970 1.000 17.31 ANISOU 1726 CA VAL 245 2108 2442 2026 -125 476 -161 ATOM 1727 CB VAL \_ 245 6.939 14.169 62.360 1.000 17.33 ANISOU 1727-CB VAL 245 2094 2473 2019 -80 340 -477 1728 CG1 VAL 245 6.551 15.334 63.286 1.000 25.25 ATOM ANISOU 1728 CG1 VAL 245 2217 ATOM 1729 CG2 VAL 245 7.252 ANISOU 1729 CG2 VAL 245 3070 ATOM 1730 C VAL 245 7.682 2966 4410 -137 1939 -1248245 7.252 14.713 60.966 1.000 21.49 245 3070 2538 2556 -180 313 271 245 7.682 245 2123 12.768 64.327 1.000 18.29 ANISOU 1730 C VAL 2689 2137 -443 508 -711731 0 VAL 245 6.765 11.945 64.429 1.000 18.62 ANISOU 1731 O VAL 245 1810 2174 3089 -15 451 254 ALA 246 8.385 ATOM 1732 N 13.202 65.369 1.000 21.54 ANISOU 1732 N ALA 246 2813 3045 2327 -591 -407 9 0 7 ATOM 1733 CA ALA 246 8.133 12.701 66.719 1.000 25.10 ANISOU 1733 CA ALA 246 4596 2562 2379 94 - 225 9 9 7 1734 CB ALA 246 9.424 ATOM 12.723 67.537 1.000 29.82 ANISOU 1734 CB ALA 246 5381 3408 2540 402 -889 1 3 2 5 MOTA 1735 C ALA 246 7.080 13.545 67.412 1.000 31.20 ANISOU 1735 C ALA 246 5079 4143 2632 314 280 428 ATOM 1736 0 ALA 246 6.876 14.714 67.052 1.000 32.39 ANISOU 1736 O ALA 246 4706 3748 3853 567 1247 - 66 1737 N ATOM ALA 247 6.429 12.973 68.413 1.000 37.30 ANISOU 1737 N ALA247 5548 5498 3126 92 640 8 3 5 1738 CA ALA 247 5.585 13.794 69.271 1.000 40.42 ANISOU 1738 CA ALA 247 5434 6048 3878 15 1313 8 5 0 MOTA ALA 247 6.289 1739 C 14.132 70.578 1.000 42.17

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ANISOU 1739 C
              ALA 247 6495
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                                       3636 -823 1720 3 4 1
       1740 O
              ALA 247 7.048
                                13.338 71.136 1.000 41.63
ANISOU 1740 O
               ALA 247 5811
                               6371
                                       3637
                                              -1631 804 425
       1741 CB ALA 247 4.280
ATOM
                               13.067 69.525 1.000 47.17
ANISOU 1741 CB
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                    247 5186
                               9059
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                                              -520 523 2683
ATOM
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               SER
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               SER
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       1743 CA
ATOM
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                    257 1.214
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                    257 2792
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ATOM
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                                22.914 68.992 1.000 28.16
ANISOU 1744 CB
                    257 2655
               SER
                                              -238 -90 -1071
                                4473
                                       3572
ATOM
       1745 OG
               SER
                    257 0.491
                                24.251 69.074 1.000 51.32
ANISOU 1745 OG
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                    257 8516
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               SER
       1746 C
                    257 2.259
                                22.389 68.034 1.000 26.19
ANISOU 1746 C
               SER
                    257 2537
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     1747 0
MOTA:
               SER
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ANISOU 1747 O
               SER
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ATOM
       1748 N
               ARG
                    258 2.022
                               22.123 66.763 1.000 26.04
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               ARG
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ATOM 1749 CA ARG
ANISOU 1749 CA ARG
                    258 2.982
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                    258 2606
                               4735
                                       2466
                                              73 - 338 - 197
ATOM
       1750 C
                    258 2.321
258 2374
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               ARG
ANISOU 1750 C
               ARG
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                    258 1.288
258 2600
       1751 0
                                21.967 64.131 1.000 19.23
ATOM
               ARG
ANISOU 1751 O
               ARG
                                2819
                                       1888
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MOTA
       1752 CB ARG
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ANISOU 1752 CB ARG
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                                5052
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       1753 CG
ATOM
              ARG
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ANISOU 1753 CG
              ARG
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      1754 CD
ATOM
              ARG
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                              19.746 64.499 1.000 30.38
ANISOU 1754 CD
               ARG
                   258 3812
                               4423
                                       3309
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                                                   341 - 16
                   258 6.433
ATOM
       1755 NE
               ARG
                              19.909 63.581 1.000 29.43
                   258 3990
ANISOU 1755 NE
               ARG
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      1756 CZ
ATOM
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                               19.389 62.359 1.000 25.02
ANISOU 1756 CZ
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               ARG
                    258 2540
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      1757 NH1 ARG
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ANISOU 1757 NH1 ARG
                    258 2105
                                2607
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                                              359
                                                    315 289
       1758 NH2 ARG
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ANISOU 1758 NH2 ARG
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ANISOU 1759 N
               THR
                   259 2010
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                                       2013
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                                       2121
                                              -533 43 -685
               THR
       1761 CB
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ANISOU 1761 CB
      1761 CB THR
1762 OG1 THR
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       1763 CG2 THR
ATOM
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ANISOU 1763 CG2 THR
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       1764 C
                    259 3.702
               THR
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ANISOU 1764 C
                    259 2035
               THR
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MOTA
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ANISOU 1766 N
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ATOM
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ATOM
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- 148 -
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MOTA
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ANISOU 1792 CE2 PHE
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                                                43 -292
      1793 CZ
               PHE
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                                24.112 44.762 1.000 12.42
ANISOU 1793 CZ
               PHE
                    263 1318
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                                        1948
                                                -138 -187 6 4 9
MOTA
      1794 C
                    263 6.636
               PHE
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ANISOU 1794 C
                PHE
                    263 1076
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                                        1223
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                                                     -14224
      1795 0
MOTA
               PHE
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ANISOU 1795 O
               PHE
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                                        1842
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MOTA
      1796 N
               PHE
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                                19.691
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ANISOU 1796 N
               PHE
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ATOM
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ANISOU 1797 CA
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                                                      -60 - 126
      1798 CB
ATOM
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ANISOU 1798 CB
                PHE
                     264 1209
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                                                      17 9
      1799 CG
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                                16.673
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ANISOU 1799 CG
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                                1647
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      1800 CD1 PHE
MOTA
                     264 6.292
                                16.236 49.139 1.000 15.38
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- 149 -ANISOU 1800 CD1 PHE 264 1467 2641 1734 -225 -8 8 7 3 ATOM 1801 CD2 PHE 264 3.986 16.433 48 808 1.000 16.96 ANISOU 1801 CD2 PHE 264 1425 3252 1769 -610 -79 958 1802 CE1 PHE 264 6.090 15.596 50.336 1.000 14.52 ANISOU 1802 CE1 PHE 264 1745 2417 1354 162 334 452 1803 CE2 PHE 264 3.755 15.796 50.019 1.000 18.04 1803 CE2 PHE 264 1747 3405 1704 -590 -109 1 0 0 8 1804 CZ PHE 264 4.817 15.354 50.779 1.000 1 2.52 1804 CZ PHE 264 1772 1536 1449 -57 227 3 3 4 1805 C PHE 264 6.535 19.038 45.533 1.000 8.98 1805 C PHE 264 1103 919 1392 143 81 -9 2 1806 C PHE 264 5.497 19.368 44.930 1.000 9.79 ANISOU 1803 CE2 PHE ATOM ANISOU 1804 CZ ATOM ANISOU 1805 C MOTA ANISOU 1806 O PHE 264 991 1190 1540 28 105 1 0 3 1807 N LEU 265 7.758 19.031 44.999 1.000 8.43 ANISOU 1807 N LEU 265 992 884 1325 173 -180 158 ATOM 1808 CA LEU 265 7.984 19.224 43.566 1.000 8.66 ANISOU 1808 CA LEU 265 883 1066 1339 63 -33 - 76 ATOM 1809 CB LEU 265 9.309 19.964 43.326 ANISOU 1809 CB LEU 265 1179 1188 1469 -225 -220 24 ATOM 1810 CG LEU 265 9.570 20.351 41.871 1.000 9.37 ANISOU 1810 CG LEU 265 1072 1009 1478 242 25 129 ATOM 1811 CD1 LEU 265 8.725 21.522 41.408 1.000 10.80 ANISOU 1811 CD1 LEU 265 1291 1004 1811 181 -114 29 ATOM 1812 CD2 LEU 265 11.048 20.684 41.678 1.000 10.87 ANISOU 1812 CD2 LEU 265 1129 1483 1519 134 43 146 ATOM 1813 C LEU 265 7.933 17.849 42.875 1.000 10.21 ANISOU 1813 C LEU 265 932 1188 1760 -6 -38 -302 1809 CB LEU 265 9.309 19.964 43.328 1.000 10.10 -225 -220 2 4 8 -114 2 9 6 ATOM 1814 O LEU 265 8.858 17.043 43.042 1.000 10.45 ANISOU 1814 O LEU 265 1388 969 1612 84 -217 107 1815 N ARG 266 6.853 17.530 42.135 1.000 10.00 ATOM ANISOU 1815 N ARG 266 1325 ANISOU 1815 N ARG 266 1325 1069 1404 -120 -222 1 5
ATOM 1816 CA ARG 266 6.572 16.198 41.628 1.000 10.50
ANISOU 1816 CA ARG 266 1219 1217 1554 -294 110 -210
ATOM 1817 CB ARG 266 5.208 15.675 42.124 1.000 10.56
ANISOU 1817 CB ARG 266 978 1460 1574 -168 -103 -105
ATOM 1818 CG ARG 266 4.965 15.894 43.609 1.000 11.24
ANISOU 1818 CG ARG 266 1337 1373 1563 -40 119 2 0 6
ATOM 1819 CD ARG 266 3.668 15.318 44.146 1.000 11.17
ANISOU 1819 CD ARG 266 1113 1567 1564 -17 -49 -11
ATOM 1820 NE ARG 266 1341 1157 1086 24 -100 -145
ATOM 1821 CZ ARG 266 1.236 15.509 43.657 1.000 9.83
ANISOU 1821 CZ ARG 266 1245 1194 1294 132 -159 - 1
ATOM 1822 NH1 ARG 266 0.961 14.567 44.572 1.000 11.20
ANISOU 1822 NH1 ARG 266 1208 1240 1806 -144 -454 2 7 2 1069 1404 -120 -222 1 5 ANISOU 1822 NH1 ARG 266 1208 1240 1806 -144 -454 2 7 2 1827 CD PRO 267 1865 13.963 40.109 1.000 12.36 1828 C2 PRO 267 1865 1132 1607 MOTA ANISOU 1827 CD PRO 267-1865 1827 CD PRO 267 1865 1132 1697 -26 -529 -1828 CA PRO 267 7.304 15.157 38.036 1.000 10.12 1828 CA PRO 267 1278 1095 1472 -129 38 -18 -529 - 192 ATOM ANISOU 1828 CA -129 38 - 185 1829 CB PRO 267 8.250 13.986 37.767 1.000 11.83 ANISOU 1829 CB PRO 267 1489 1088 1919 -72 90 -322 PRO 267 8.017 13.053 38.913 1.000 10.72 1830 CG ANISOU 1830 CG PRO 267 960 1356 1755 95 - 257 - 187

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- 150 -
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PRO 267 1330 1226 1570 -252 47 -16
PRO 267 5.030 14.421 37.934 1.000 12.03
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 ANISOU 1831 C
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                   PRO
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268 1216
268 4.810
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                   ASN
 ANISOU 1833 N
                   ASN
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                                                             -86 -129
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         1834 CA
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        1834 CA ASN 268 4.810 14.949 35.196 1.000 11.20 1834 CA ASN 268 1285 1349 1622 -167 -43 -22 1835 CB ASN 268 4.954 15.664 33.846 1.000 14.02 1836 CG ASN 268 2160 1410 1756 132 -316 2 3 1836 CG ASN 268 4.992 17.175 33.992 1.000 13.03 1837 OD1 ASN 268 4.046 17.748 34.566 1.000 16.65 1744 2673 292 -1 -159
 ANISOU 1834 CA
                                                        -167 -43 -229
 ANISOU 1835 CB
 ANISOU 1836 CG
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ANISOU 1837 OD1 ASN
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                                                2673
                                                        292 -1 -159
         1838 ND2 ASN
                        268 6.037 17.818 33.495 1.000 14.19
MOTA
ANISOU 1838 ND2 ASN
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ATOM
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1840 O ASN 268 5.715
ANISOU 1339 C
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ATOM
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ANISOU 1840 O ASN 268 1534
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ATOM
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ANISOU 1842 CA ALA 269 1432 1356 1819 -238 -29 -2
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ANISOU 1843 CB ALA 269 1439 1278 1985 -228 -183 2
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269 4.493 9.800 33.263 1.000 12.53
ANISOU 1844 C
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                                                        25 - 280 - 141
ATOM
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                   ALA
ANISOU 1845 O
                       ALA
                                                        -110 108 -188
ATOM
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                  ASP
        1846 N ASP 270 1701 1280 1378 -261 -341 -300 1847 CA ASP 270 5.214 11.378 31.113 1.000 11.92 1848 CB ASP 270 4.760 12.096 29.850 1.000 14.13 1848 CB ASP 270 1733 2038 1597 84 111 2 1 2
ANISOU 1846 N
ATOM
ANISOU 1847 CA ASP
ATOM
ANISOU 1848 CB ASP
                        270 5.050 13.568 29.777 1.000 15.98
ATOM
                  ASP
ANISOU 1849 CG
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        1850 OD1 ASP
ATOM
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ANISOU 1850 OD1 ASP
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        1851 OD2 ASP
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ANISOU 1851 OD2 ASP
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1392 1654 -398 -61 315
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        1853 O ASP
ATOM
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ANISOU 1855 CA
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271 1242 1349 1641 10 230 162
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                  PHE
        1856 CB
ATOM
                  PHE
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271 1467 1444 1722 -96 -3 18
ANISOU 1856 CB
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                                                        -96 -3 1 8 2
        1857 CG
                        271 10.385 11.992 34.597 1.000 12.77
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ANISOU 1858 CD1 PHE
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                                               1993
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        1859 CD2 PHE
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ANISOU 1859 CD2 PHE
                        84 2 5 5
MOTA
        1860 CE1 PHE
ANISOU 1860 CE1 PHE
                        1861 CE2 PHE
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ANISOU 1861 CE2 PHE 271 1537 1818 2679 -263 -675 2
ATOM 1862 CZ PHE 271 13.006 11.288 35.304 1.000 14.15
ANISOU 1862 CZ PHE 271 1166 1736 2475 7 -531 -46
ATOM 1863 C PHE 271 9.259 10.550 32.410 1.000 11.27
ANISOU 1863 C PHE 271 1359 1338 1585 75 271 3 4 8
ATOM 1864 O PHE 271 8.785 9.531 32.920 1.000 12.97
ANISOU 1864 O PHE 271 2011 1320 1596 -85 473 2 -263 -675 2 6 0 7 -531 -467 **-**85 473 2 7 9 THR 272 10.261 10.498 31.541 1.000 11.95
THR 272 1018 1503 2020 -214 300 -1865 N ANISOU 1865 N -214 300 -115 1866 CA THR 272 10.823 9.254 30.992 1.000 12.70 ANISOU 1866 CA THR 272 1615 1652 1557 132 341 146 ANISOU 1867 CB THR 272 1814 2829 1737 -595 157 -40

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ANISOU 1868 OG2 THR 272 11.200 7.976 28.856 1.000 17.002

ANISOU 1869 CG2 THR 272 2144 2857 1467 -475 538 -19

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ANISOU 1870 C THR 272 1436 1573 1559 92 603 1 3 7

ATOM 1871 O THR 272 1451 1583 2351 125 602 4 1 2

ANISOU 1871 O THR 272 1451 1583 2351 125 602 4 1 2

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ANISOU 1872 N PHE 273 1402 1585 1703 17 378 1 5 8

ATOM 1873 CA PHE 273 13.951 7.492 32.312 1.000 12.20

ANISOU 1874 CB PHE 273 13.62 1364 1909 -126 336 1 4 7

ANISOU 1874 CB PHE 273 13.951 7.514 33.861 1.000 12.37

ANISOU 1875 CG PHE 273 13.98 6.528 34.491 1.000 11.65

ANISOU 1876 CD1 PHE 273 13.98 1631 1396 -367 42 -2 15

ANISOU 1876 CD1 PHE 273 11.684 6.889 34.773 1.000 14 11

ATOM 1877 CD2 1867 CB THR ATOM 29.450 1.000 16.79 272 10.679 9.281 -475 538 -194 273 1531 2214 1614 -336 293 - 62 273 13.409 5.245 34.803 1.000 13.20 273 2024 1639 1352 -358 339 -273 10.793 5.993 35.323 1.000 13.25 273 1536 2081 1418 -98 447 4 ATOM 1877 CD2 PHE ANISOU 1877 CD2 PHE -358 339 ~ 9 1878 CE1 PHE ANISOU 1878 CE1 PHE ANISOU 1878 CE1 PHE 273 1536 2081 1418 -98 447 4 ATOM 1879 CE2 PHE 273 12.530 4.329 35.327 1.000 13.39 ANISOU 1879 CE2 PHE 273 1529 1905 1654 -224 140 2 447 4 2 ATOM 1880 CZ PHE 273 11.227 4.706 35.604 1.000 14.75 ANISOU 1880 CZ PHE 273 1444 2260 1902 -90 -186 2 7 5 PHE 273 14.423 6.135 31.795 1.000 12.45
PHE 273 1278 1526 1927 -120 317 - 3 1
PHE 273 13.645 5.311 31.291 1.000 11.95
PHE 273 1590 1580 1370 -137 226 - 1 3 ATOM ANISOU 1881 C ATOM 1882 0 ANISOU 1882 O PHE 273 1590 1580 1370 -137 226 -13 ATOM 1883 N SER 274 15.717 5.854 31.952 1.000 12.07 ANISOU 1883 N SER 274 1270 1640 1677 -29 558 3 5 3 ATOM 1884 CA SER 274 16.335 4.586 31.604 1.000 14.39 ANISOU 1884 CA SER 274 1583 1534 2349 43 707 3 8 4 ATOM 1885 CB SER 274 17.845 4.771 31.438 1.000 14.49 ANISOU 1885 CB SER 274 1578 1727 2202 213 695 3 2 9 ATOM 1886 OG SER 274 18.564 3.558 31.424 1.000 14.97 ANISOU 1886 OG SER 274 1763 1848 2078 349 348 -13 ATOM 1887 C SER 274 16.100 3.505 32.666 1.000 13.12 ANISOU 1887 C SER 274 16.100 3.505 32.666 1.000 13.12 ANISOU 1888 O SER 274 16.438 3.700 33.834 1.000 13.50 ANISOU 1888 O SER 274 1493 1518 2116 -65 119 1 5 ATOM 1889 N VAL 275 15.533 2.359 32.271 1.000 11.90 ANISOU 1882 O VAL 275 15.533 2.359 32.271 1.000 11.90 1889 N ANISOU 1889 N VAL 275 1476 1618 1427 -110 490 195 ATOM 1890 CA 275 15.283 1.254 33.180 1.000 11.41 VAL ANISOU 1890 CA VAL 275 1708 1424 -8 286 7 6 1204 ATOM 1891 CB VAL 275 14.346 0.198 32.543 1.000 12.74 ANISOU 1891 CB VAL 275 1732 1300 1809 62 164 - 16

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- 152 -
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                 VAL
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        1895 0
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                 VAL
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276 1411 2689 2275
        1902 0
 ATOM
                 PRO
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MOTA
                LEU
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ANISOU 1905 CB
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ATOM
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ANISOU 1907 CD1 LEU
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ANISOU 1908 CD2 LEU
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277 19.411 2.989 36.430 1.000 16.55
277 1975 1885 2430 -218 211 -
277 19.997 3.116 37.517 1.000 19.19
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ATOM
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ATOM
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ATOM
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MOTA
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MOTA
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ANISOU 1922 CZ ARG 279 4486 3045 4948 -475 448 -1
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ARG 279 3764 3102 3325 -1987 -1467 13

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GLU 280 5144 5703 4221 -64 1339 - 6
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  ATOM
                                 1931 CD
ATOM 1931 CD GLU 280 23.698 0.341 35.590 1.000 39.66 ANISOU 1931 CD GLU 280 5144 5703 4221 -64 1339 - 6 ATOM 1932 OE1 GLU 280 3464 5891 5710 334 574 1639 ATOM 1933 OE2 GLU 280 23.489 -0.294 34.519 1.000 41.55 ANISOU 1933 OE2 GLU 280 2527 6747 3781 2245 -184 10 2 ATOM 1934 C GLU 280 21.984 1.188 40.266 1.000 19.68 ANISOU 1934 C GLU 280 23.031 1.142 40.958 1.000 25.69 ANISOU 1935 O GLU 280 23.031 1.142 40.958 1.000 25.69 ANISOU 1936 N CYS 281 20.943 1.980 40.565 1.000 18.57 ANISOU 1936 N CYS 281 20.943 1.980 40.565 1.000 18.57 ANISOU 1937 CA CYS 281 21.098 2.762 41.806 1.000 23.83 ANISOU 1937 CA CYS 281 21.098 2.762 41.806 1.000 23.83 ANISOU 1937 CA CYS 281 21.098 2.762 41.806 1.000 25.40 ANISOU 1938 CB CYS 281 3222 2647 3184 -1189 176 -122 ATOM 1938 CB CYS 281 3228 2655 3718 -426 368 -46 ATOM 1939 SG CYS 281 19.587 4.904 40.763 1.000 25.40 ANISOU 1939 SG CYS 281 19.587 4.904 40.763 1.000 27.05 ANISOU 1940 C CYS 281 1377 1604 4295 -522 -37 -794 ATOM 1940 C CYS 281 1377 1604 4295 -522 -37 -794 ANISOU 1940 C CYS 281 1377 1604 3475 109 -6-546 ATOM 1941 O CYS 281 1377 1604 3475 109 -6-546 ATOM 1941 O CYS 281 1377 1604 3475 109 -6-546 ATOM 1941 O CYS 281 1377 1604 3475 109 -6-546 ATOM 1942 N GLY 282 19.447 1.245 42.794 1.000 15.23 ANISOU 1942 N GLY 282 19.447 1.245 42.794 1.000 15.61 ANISOU 1943 CA GLY 282 1667 1597 2572 3 -58 -436 ATOM 1944 C GLY 282 1665 1973 2394 6 -331 -266 ATOM 1944 C GLY 282 17.246 0.519 43.727 1.000 15.61 ANISOU 1944 C GLY 282 17.246 0.519 43.727 1.000 13.75 ANISOU 1944 C GLY 282 17.246 0.519 43.727 1.000 13.75 ANISOU 1944 C GLY 282 17.246 0.519 43.727 1.000 13.75 ANISOU 1944 C GLY 282 17.246 0.519 43.727 1.000 13.75 ANISOU 1944 C GLY 282 1635 1562 2029 -270 -4465 -78
  ANISOU 1931 CD
ANISOU 1943 CA GLY 282 1565 1973 2394 6 -331 -266 ATOM 1944 C GLY 282 17.246 0.519 43.727 1.000 13.75 ANISOU 1944 C GLY 282 1635 1562 2029 -270 -446 - 78 ATOM 1945 O GLY 282 16.585 0.012 44.639 1.000 14.99 ANISOU 1945 O GLY 282 16.585 0.012 44.639 1.000 14.99 ANISOU 1946 N PHE 283 16.744 1.009 42.582 1.000 12.65 ANISOU 1946 N PHE 283 1434 1803 1570 -200 18 -252 ATOM 1947 CA PHE 283 15.292 0.886 42.374 1.000 11.80 ANISOU 1947 CA PHE 283 14.839 1.890 41.295 1.000 14.13 ANISOU 1948 CB PHE 283 14.839 1.890 41.295 1.000 14.13 ANISOU 1949 CG PHE 283 14.906 3.351 41.757 1.000 12.63 ANISOU 1949 CG PHE 283 14.906 3.351 41.757 1.000 12.63 ANISOU 1949 CG PHE 283 13.851 3.928 42.409 1.000 13.45 ANISOU 1950 CD1 PHE 283 16.037 4.111 41.519 1.000 13.15 ANISOU 1951 CD2 PHE 283 16.037 4.111 41.519 1.000 13.15 ANISOU 1951 CD2 PHE 283 1567 1135 2295 142 -41 -99 ATOM 1952 CE1 PHE 283 13.903 5.248 42.839 1.000 15.61
                                                                                            283 13.903 5.248 42.839 1.000 15.61
                                 1952 CE1 PHE
  ANISOU 1952 CE1 PHE
                                                                                             283 2111 1649 2171
                                                                                                                                                                                                                    -202 484 -617
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- 154 -

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1953 CE2 PHE 283 16.112 5.432 41.963 1.000 12.60
   ANISOU 1953 CE2 PHE 283 1783 937 2068 32 -18 264
                       1954 CZ PHE 283 15.040 5.993 42.641 1.000 13.37
   ANISOU 1954 CZ PHE 283 1863 865 2352 187 -149 1 3
ATOM 1955 C PHE 283 14.915 -0.534 41.972 1.000 11.23
ANISOU 1955 C PHE 283 1527 974 1765 63 -172 6 5
                                            PHE 283 15.471 -1.071 40.990 1.000 13.24

PHE 283 1249 1428 2355 175 -120 -1

ASP 284 13.998 -1.130 42.712 1.000 12.31

ASP 284 1607 1333 1736 -268 -312 8

ASP 284 13.589 -2.528 42.527 1.000 12.48
                       1956 0
   ANISOU 1956 O
                                                                                            1428 2355 175 -120 - 361
                      1957 N
   ATOM
   ANISOU 1957 N
                                                                                                                                        -268 -312 8 7
                      1958 CA
   -148 -543 3 5 0
                     1960 CG ASP 284 2014 1145 1656 -50 -406 1
1960 CG ASP 284 13.261 -4.667 43.909 1.000 13.40
1961 OD1 ASP 284 2077 1171 1843
                                                                                                                                        -50. -406 1 3 5
   ANISOU 1960 CG
                     1960 CG ASP 284 2077 1171 1843 110 -419 3
1961 OD1 ASP 284 13.861 -5.246 42.974 1.000 14.98
ANISOU 1960 CG ASP 284 2077 1171 1843 110 -419 36 3 ATOM 1961 OD1 ASP 284 13.861 -5.246 42.974 1.000 14.98 ANISOU 1961 OD1 ASP 284 1956 1094 2640 -87 11 6 0 ATOM 1962 OD2 ASP 284 12.762 -5.306 44.883 1.000 15.79 ANISOU 1962 OD2 ASP 284 22494 1539 1966 -330 -446 43 8 ATOM 1963 C ASP 284 12.478 -2.641 41.510 1.000 10.82 ATOM 1964 O ASP 284 1238 1387 1487 -205 -99 12 3 ATOM 1964 O ASP 284 1331 175 2159 -209 48 19 1 ATOM 1965 N VAL 285 12.751 -2.154 40.308 1.000 11.32 ANISOU 1965 N VAL 285 12.751 -2.154 40.308 1.000 11.32 ANISOU 1966 CA VAL 285 12.751 -2.154 40.308 1.000 11.32 ATOM 1966 CA VAL 285 11.748 -2.062 39.260 1.000 11.45 ATOM 1966 CA VAL 285 1468 1384 1500 39 -219 -15 ATOM 1966 CA VAL 285 1468 1384 1500 39 -219 -15 ATOM 1966 CA VAL 285 1412 1523 1465 -388 -428 -8 ATOM 1969 CG2 VAL 285 12.278 0.362 38.679 1.000 15.02 ATOM 1969 CG2 VAL 285 1909 1443 2615 -1.59 309 44 7 ANISOU 1969 CG2 VAL 285 11.424 -3.431 38.642 1.000 15.70 ANISOU 1970 C VAL 285 12.267 ANISOU 1971 O VAL 285 12.267 ANISOU 1972 N SER 286 10.168 -3.523 38.248 1.000 11.09 ANISOU 1972 N SER 286 10.168 -3.523 38.248 1.000 11.09 ANISOU 1972 N SER 286 10.168 -3.523 38.248 1.000 11.09 ANISOU 1972 N SER 286 10.168 -3.523 38.248 1.000 11.09 ANISOU 1972 N SER 286 10.168 -3.523 38.248 1.000 11.09 ANISOU 1972 N SER 286 10.168 -3.523 38.248 1.000 11.09 ANISOU 1972 N SER 286 10.168 -3.523 38.248 1.000 11.09 ANISOU 1973 CA SER 286 10.168 -3.523 37.510 1.000 11.32
                                                                                                                   1843 110 -419 3 6 3
                     1972 N SER 286 1116
1973 CA SER 286 9.558
                                                                                                                  1489
                                                                                                                                       -76 96 7
  ATOM
                                                                                             -4.622 37.510 1.000 11.32
 ANISOU 1973 CA SER 286 1104
                                                                                           1479
                                                                                                                   1718
                                                                                                                                       -41 -274 2 5 2
                     1974 CB SER 286 8.483 -5.292 38.344 1.000 9.88
  ATOM
 ANISOU 1974 CB SER 286 1328 1141 1285 72 -207 7 0
ANISOU 1975 OG SER 286 7.570 -4.361 38.905 1.000 11.34
ANISOU 1975 OG SER 286 1391 1188 1729 147 -153 7
ATOM 1976 C SER 286 9.019
ANISOU 1976 C SER 286 9.019
ANISOU 1977 O SER 286 7.829
ANISOU 1977 O SER 286 1223
ATOM 1978 N LEU 287 9.926
ANISOU 1978 N LEU 287 9.926
ANISOU 1979 CA LEU 287 9.654
ANISOU 1979 CA LEU 287 1622
ATOM 1980 CB LEU 287 10.145
                                                                                                                                        147 -153 7 5
                                           LEU 287 1622 1558 1605 -366 94 18 4
LEU 287 10.145 -1.452 34.210 1.000 12.91
 ATOM
                     1980 CB
 ANISOU 1980 CB
                                           LEU 287 1716 1591 1597 -373 -95 2 7
LEU 287 9.452 -0.590 35.264 1.000 12.96
 ATOM
                     1981 CG
 ANISOU 1981 CG
                     1981 CG LEU 287 1182 1848 1895 -407 -51 -170 1982 CD1 LEU 287 10.229 0.708 35.484 1.000 13.34
 ATOM
 ANISOU 1982 CD1 LEU
                                                          287 1644 1108 2318 -38 -124 2
287 8.006 -0.248 34.914 1.000 14.56
                                                                                                                2318 -38 -124 2 2 3
 ATOM 1983 CD2 LEU
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		4.5.5	-
ANISCU 1983 CD2 ATOM 1984 C ANISCU 1984 C ANISCU 1985 O ANISCU 1985 O ATOM 1986 N ANISCU 1986 N ATOM 1987 CA ANISCU 1987 CA ANISCU 1988 CB ATOM 1988 CB ATOM 1989 CG ANISCU 1989 CG ANISCU 1989 CG ANISCU 1989 CG ANISCU 1990 OD1 ANISCU 1991 OD2 ANISCU 1991 OD2 ATOM 1992 C	LEU 287 10.319 LEU 287 1837 LEU 287 11.529 LEU 287 1779 ASP 288 9.531 ASP 288 2080 ASP 288 10.079 ASP 288 2029 ASP 288 8.979 ASP 288 2722 ASP 288 2722 ASP 288 2467 ASP 288 10.447 ASP 288 2812	-155- 1548	36 -550 318 1.000 12.63 -233 248 354 1.000 16.68 -292 390 -149 1.000 13.91 4 223 2 27 1.000 15.50 -122 605 153 1.000 17.00 -250 362 - 2 1.000 19.30 173 243 - 377 1.000 25.95 501 -239 - 783 1.000 31.76 1266 -849 - 1154 1.000 17.08
ANISOU 1994 N ATOM 1995 CA ANISOU 1996 C ANISOU 1996 C ANISOU 1997 O ANISOU 1997 O ANISOU 1998 N ANISOU 1998 N ANISOU 1999 CA ANISOU 1999 CA ANISOU 2000 CB ATOM 2001 CG ANISOU 2001 CG ANISOU 2001 CG ANISOU 2002 CD ATOM 2002 CD ATOM 2003 OE1 ANISOU 2004 OE2 ANISOU 2004 OE2 ANISOU 2005 C ANISOU 2006 O ANISOU 2006 O ANISOU 2007 N ANISOU 2008 CA ANISOU 2007 N ANISOU 2008 CA ANISOU 2009 CB ANISOU 2009 CB ANISOU 2010 OG1 ANISOU 2011 CG2 ANISOU 2011 CG2 ANISOU 2012 C ANISOU 2013 O ANISOU 2013 O ANISOU 2013 O	GLY 289 13.414 GLY 289 3230 GLU 290 13.562 GLU 290 2665 GLU 290 14.716 GLU 290 2470 GLU 290 15.579 GLU 290 16.071 GLU 290 3251 GLU 290 3019 GLU 290 16.812 GLU 290 3019 GLU 290 16.812 GLU 290 3019 GLU 290 16.336 GLU 290 6893 GLU 290 6893 GLU 290 14.406 GLU 290 2512 GLU 290 15.260 GLU 290 2074 THR 291 13.232 THR 291 12.792 THR 291 12.792 THR 291 12.766 THR 291 1756	3699	-610 752 5 1 1 1.000 21.65 -1163 71 6 2 6 1.000 22.09 -738 -23 2 4 3 1.000 20.34 -918 124 1 4 7 1.000 16.48 5 222 - 4 4 5 1.000 16.94 81 411 - 4 8 4 1.000 20.26 414 863 - 2 3 9 1.000 24.53 664 1218 - 6 1 2 1.000 27.91 989 940 - 2 5 1 1.000 35.13 963 - 85 - 8 7 7 1.000 43.76 -30 - 748 5 9 8 1.000 15.25 50 418 - 2 6 2 1.000 15.72 78 346 - 5 1 9 1.000 15.72 78 346 - 5 1 9 1.000 18.67 -361 769 3 3 6 1.000 22.93 445 78 1 4 6 1.000 21.82 357 1450 9 0 2 1.000 12.86 47 305 2 1 9 1.000 16.13 -303 750 - 4 3 1

- 156 -ATOM 2014 N ALA 292 11.037 3.791 30.542 1.000 12.41 ANISOU 2014 N ALA 292 1495 1363 1859 -2 256 7 7 ATOM 2015 CA ALA 292 9.746 3.839 31.202 1.000 11.57 ANISOU 2015 CA ALA 292 1362 1257 1779 -213 153 3 ATOM 2016 CB ALA 292 9.718 2.954 32.439 1.000 12.62 ANISOU 2016 CB ALA 292 1768 1245 1784 100 357 4 ATOM 2017 C ALA 292 9.385 5.255 31.614 1.000 10.32 ANISOU 2017 C ALA 292 1317 1335 1270 -181 99 5 4 -213 153 3 7 ALA 292 1317 ANISOU 2017 C ALA 292 1317 1335 1270 -181 99 5 4 ALA 292 10.266 6.134 31.701 1.000 10.97 MOTA 2018 0 ALA 292 1389 1138 1641 -146 279 1 0 4 THR 293 8.091 5.445 31.882 1.000 12.32 THR 293 1486 1547 1647 -314 563 -28 ANISOU 2018 O 2019 N MOTA THR 293 1486 1547 1647 -314 563 -284
THR 293 7.626 6.715 32.421 1.000 12.28
THR 293 1717 1460 1489 -168 337 -200
THR 293 6.352 7.215 31.733 1.000 13.27
THR 293 2128 1182 1730 -258 -159 -284
THR 293 5.317 6.237 31.911 1.000 13.85 ANISOU 2019 N ATOM 2020 CA ANISOU 2020 CA ATOM 2021 CB ANISOU 2021 CB 2022 OG1 THR ATOM ANISOU 2022 OG1 THR 293 1831 1217 2216 8 -131 7 4 2023 CG2 THR 293 6.474 7.303 30.212 1.000 13.72 ANISOU 2023 CG2 THR 1683 1738 -252 55 6.635 33.937 1.000 10.58 1533 12 447 9 293 1791 -252 -56 -405 293 7.363 2024 C THR ANISOU 2024 C ATOM 2025 O THR 293 1439 THR 293 7.211 34.553 1.000 10.29 5.576 ANISOU 2025 O THR 293 1049 THR 293 1049 1102 1758 -56 93 1 18 PHE 294 7.243 7.810 34.569 1.000 11.53 PHE 294 1794 1093 1494 -307 306 -6 PHE 294 6.806 7.939 35.950 1.000 10.41 PHE 294 1432 1061 1463 -174 125 -1 PHE 294 6.709 9.426 36.336 1.000 12.25 PHE 294 1930 1030 1694 -164 292 -6 PHE 294 6.270 9.658 37.770 1.000 12.77 PHE 294 1880 1136 1837 -103 178 -4 PHE 294 7.123 9.462 38.839 1.000 14.73 PHE 294 1976 1893 1727 -539 161 -1 1102 1758 -56 93 1 1 8 ATOM 2026 N ANISOU 2026 N -307 306 - 66 ATOM 2027 CA ANISOU 2027 CA -174 125 -162 2028 CB ATOM ANISOU 2028 CB 1030 1694 -164 292 -64 9.658 37.770 1.000 12.77 2029 CG ATOM 2029 CG PHE 294 1880 1136 1837 -103 178 -427 2030 CD1 PHE 294 7.123 9.462 38.839 1.000 14.73 2030 CD1 PHE 294 1976 1893 1727 -539 161 -132 2031 CD2 PHE 294 4.989 10.068 38.056 1.000 16.59 2031 CD2 PHE 294 2180 1923 2199 348 386 -492 2032 CE1 PHE 294 6.726 9.673 40.144 1.000 14.36 2032 CE1 PHE 294 1500 2020 1830 505 280 -118 ANISOU 2029 CG MOTA ANISOU 2030 CD1 PHE ATOM ANISOU 2031 CD2 PHE ATOM ANISOU 2032 CE1 PHE 294 1598 2028 1830 -505 280 -118 2033 CE2 PHE ATOM 294 4.575 10.275 39.345 1.000 16.75 ANISOU 2033 CE2 PHE 294 2214 2062 2087 692 144 - 294 5.426 10.065 40.413 1.000 15.17 2062 2087 692 144 -602 2034 CZ ATOM PHE ANISOU 2034 CZ PHE 294 2040 1426 2296 327 97 - 135 ATOM 2035 C PHE 294 5.484 7.195- 36.172 1.000 10.89 ANISOU 2035 C PHE 294 1401 1200 1536 -155 78 1 3 7 ATOM 2036 O 294 5.325 PHE 6.425 37.125 1.000 10.67 ANISOU 2036 O PHE 294 1396 1297 1360 90 337 1 0 5 ATOM 2037 N GLN295 4.487 7.355 35.299 1.000 10.62 ANISOU 2037 N GLN 295 1399 1187 1450 -18 88 - 24 ATOM 2038 CA  ${ t GLN}$ 295 3.217 6.612 35.393 1.000 11.31 ANISOU 2038 CA GLN 295 1433 1205 1660 -96 120 - 321 ATOM 2039 CB ANISOU 2039 CB ATOM 2040 CG GLN295 2.284 7.053 34.254 1.000 11.66 GLN 295 1425 GLN 295 0.951 1053 1953 -25 63 - 141 6.360 34.200 1.000 11.05 295 1573 295 0.052 ANISOU 2040 CG GLN1011 1614 -93 -118 1 8 MOTA 2041 CD GLN6.843 33.087 1.000 11.35 ANISOU 2041 CD GLN 295 1592 1326 1395 173 57 - 13 2042 OE1 GLN 295 0.349 7.823 32.378 1.000 15.06 ANISOU 2042 OE1 GLN 1589 1825 110 7 3 7 9 295 2306 295 -1.053 6.153 32.914 1.000 13.90 2043 NE2 GLN ANISOU 2043 NE2 GLN 295 1511 1757 2015 156 -282 2 295 3.412 5.107 35.389 1.000 10.12 156 -282 2 0 8 MOTA 2044 C GLN

	•			457		
ANISOU 20	44 C	GLN	295 1154	- 157 - 1203	1486	21 160 - 191
ATOM 20	45 0	GLN	295 2.827	4.309	36.128	1.000 11.82
ANISOU 20	45 O 46 N	GLN ASP	295 1264 296 4.267	1542 4.558	1686 34.538	-107 41 1 3 7 1.000 9 . 3 5
ANISOU 20		ASP	296 1076	1056	1422	-118 -75 -275
	47 CA	ASP	296 4.655	3.172	34.416	1.000 9 . 9 1
ANISOU 20 ATOM 20	47 CA 48 CB	ASP ASP	296 1241 296 5.699	1139 2.852	1387	56 60 - 243
ANISOU 20		ASP	296 1315	1156	33.347 1429	1.000 10.26 113 132 - 36
	19 CG	ASP	296 5.343	2.981	31.885	1.000 11.42
ANISOU 20	19 CG 50 OD1	ASP	296 1357 296 4.143	1578 2.904	1405	358 121 -199
ANISOU 20	50 OD1	ASP	296 1511	1744	31.531 1997	1.000 13.82 149 -209 - 62
ATOM 20	51 OD2	ASP	296 6.282	3.151	31.047	1.000 13.48
ANISOU 20: ATOM 20!	22 C	ASP	296 1802 296 5.175	1758 2.682	1564 35.770	228 364 7 3 1.000 10.31
ANISOU 203	52 C	ASP	296 1416	1141	1361	16 91 - 198
ATOM 205 ANISOU 205	53 (	ASP	296 4.852	1.551	36.197	1.000 11.40
	54 N	ASP TRP	296 1428 297 6.004	1452 3.484	1453 36.441	-288 32 3 5 1.000 10.88
ANISOU 20	54 N	TRP	297 1752	1144	1238	-161 11 5 5
ATOM 203 ANISOU 203	55 CA	TRP TRP	297 6.646 297 1768	3.104	37.685	1.000 11.26
	6 CB	TRP	297 1768	1215 3.999	1294 37.890	-217 -57 4 5 1.000 10.31
ANISOU 205		TRP	297 1387	1417	1112	-87 213 120
ATOM 205 ANISOU 205	57 CG 57 CG	TRP TRP	297 8.621 297 1456	3.651 1394	39.172 1324	1.000 10.98 164 -29 - 43
ATOM 205	8 CD2	TRP	297 9.082	4.534	40.202	1.000 12.49
ANISOU 205 ATOM 205	8 CD2 89 CE2	TRP	297 1255	1729	1761	75 - 298 - 197
ANISOU 20	59 CE2	TRP	297 9.692 297 1860	3.755 2049	41.201 2202	1.000 16.08 -294 -977 4 9
ATOM 206	50 CE3	TRP	297 9.040	5.910	40.379	1.000 17.41
ANISOU 206 ATOM 206	50 CE3 51 CD1	TRP	297 2778 297 8.969	1740 2.400	2096	-388 -916 - 234
ANISOU 206	51 CD1	TRP	297 1617	1518	39.589 2025	1.000 13.58 0 -664 114
ATOM 206 ANISOU 206	2 NE1	TRP	297 9.614	2.444	40.808	1.000 16.12
ATOM 200	53 CZ2	TRP	297 2165 297 10.243	1909 4.320	2051 42.341	-22 -873 2 2 0 1.000 19.85
ANISOU 20	33 CZ2	TRP	297 2756	2383	2404	-951 -1337 267
ATOM 206 ANISOU 206	54 CZ3	TRP	297 9.586 297 4215	6.466	41.515	1.000 23.40
	55 CH2		297 4215	2030 5-670	2645 42.486	-1001 -1757 - 77 1.000 21.51
ANISOU 206	55 CH2		297 3178	2457	2537	-910 -1473 - 51
ATOM 206 ANISOU 206	66 C	TRP TRP	297 5.700 297 1172	3.138 1448	38.882 1329	1.000 10.39 -280 -237 3 9 1
ATOM 206	57 0	TRP	297 5.574	2.159	39.639	-280 -237 3 9 1 1.000 13.52
ANISOU 200 ATOM 200	57 O 58 N	TRP	297 1748	1830	1557	32 -91 7 0 3
ANISOU 206		ILE	298 5.033 298 1400	4.272 1710	39.079 1480	1.000 12.08 -49 83 4 5 1
ATOM 200	59 CA	ILE	298 4.223	4.521	40.272	1.000 13.43
ANISOU 200 ATOM 201	59 CA 70 CB	ILE	298 1301	2484	1317	-199 -158 - 33
ANISOU 20		ILE	298 4.370 298 1877	5.988 2908	40.689 1661	1.000 16.97 -1000 214 -630
ATOM 20	71 CG2	ILE	298 3.538	6.423	41.876	1.000 22.01
ANISOU 201 ATOM 201	/1 CG2 72 CG1	ILE	298 3980 298 5.847	3121 6.253	1263	-233 546 -339 1.000 27.10
ANISOU 20	72 CG1	ILE	298 2588	5151	41.037 2557	-2140 -708 9 7
ATOM 20° ANISOU 20°	73 CD1	ILE	298 6.365	5.522	42.266	1.000 43.13
	73 CD1	ILE	298 5185 298 2.772	8299 4.116	2904 40.131	-3717 -3055 7 0 8 1.000 1 0 . 9 4
ANISOU 20		ILE	298 1350	1652	1156	-165 -79 9 6

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- 158 -
               2075 O ILE 298 2.137 3.844 41-155 1.000 12.67
2076 N GLY 299 2.267 4.077 38.897 1.000 10.14
2076 N GLY 299 1412 1057 1384 -51 -377 201
2077 CA GLY 299 0.866 3.822 38.695 1.000 10.72
2078 C GLY 299 1335 1084 1655 0 -229 -206
2078 C GLY 299 0.049 5.054 38.369 1.000 12.05
2079 C GLY 299 1422 1293 1864 105 -292 0
2079 C GLY 299 1422 1293 1864 105 -292 0
2079 C GLY 299 1917 1199 1866 174 80 -23
2080 N GLY 300 -1.268 4.931 38.490 1.000 13.11
2080 N GLY 300 1393 1531 2363 182 -410 -223
2081 CA GLY 300 1524 1471 2331 217 -563 -33 6
2082 C GLY 300 940 1603 2004 67 -488 -295
2082 C GLY 300 940 1603 2004 67 -488 -295
2083 O GLY 300 1219 1408 1515 -37 -203 -1 34
2084 N ASN 301 -2.587 7.015 39.074 1.000 11.97
2085 CA ASN 301 -2.195 7.915 41.323 1.000 13.39
2086 CB ASN 301 -3.047 7.301 42.427 1.000 17.60
2087 CG ASN 301 -4.021 8.196 43.108 1.000 19.15
2087 CG ASN 301 -4.021 8.196 43.108 1.000 19.15
               2075 O ILE 298 2.137 3.844 41-155 1.000 12.67
  ANISOU 2075 O
  ANISOU 2076 N
  ATOM
  ANISOU 2077 CA GLY
  ATOM
 ANISOU 2078 C
 ATOM
 ANISOU 2079 O
 MOTA
 ANISOU 2080 N
 ATOM
 ANISOU 2081 CA GLY
 ATOM
 ANISOU 2082 C
 ATOM
 ANISOU 2083 O
ATOM 2084 N
 ANISOU 2084 N
 ANISOU 2085 CA ASN
ANISOU 2086 CB ASN 301 1391 2869 2426 -9 326 2 28

ATOM 2087 CG ASN 301 -4.021 8.196 43.108 1.000 19.15

ATOM 2087 CG ASN 301 2549 2827 1900 805 59 3 7 7

ATOM 2088 OD1 ASN 301 -5.072 8.606 42.591 1.000 15.47

ANISOU 2088 OD1 ASN 301 1258 2340 2280 -253 339 -

ATOM 2089 ND2 ASN 301 -3.661 8.510 44.367 1.000 29.28

ATOM 2090 C ASN 301 -0.862 8.331 41 014
                                                                                                                   805 59 3 7 7
                                                                                                                   -253 339 - 8
                                                                                                                   1521 -850 -885
ATOM 2090 C ASN 301 -0.862 8.331 41.914 1.000 11.31 ANISOU 2090 C ASN 301 1436 1669 1194 1 1 -168 ATOM 2091 O ASN 301 -0.033 7.456 42.221 1.000 12.03 ANISOU 2091 O ASN 301 1483 1548 1542 -151 -279 8 2 ATOM 2092 N TYR 302 -0.634 9.628 42.133 1.000 11.53 ANISOU 2092 N TYR 302 1186 1584 1611 -61 26102 ATOM 2093 CA TYR 302 0.573 10.046 42.838 1.000 11.90 ANISOU 2093 CA TYR 302 1260 1395 1865 5 -212 225 ATOM 2094 CB TYR 302 0.657 11.589 43.036 1.000 13.14 ANISOU 2094 CB TYR 302 1768 1404 1820 -273 190 181 ATOM 2095 CG TYR 302 1.082 12.287 41.750 1.000 10.88 ANISOU 2095 CG TYR 302 1395 1347 1393 -321 2 -153
                                      ASN 301 -0.862 8.331 41.914 1.000 11.31
                                      TYR 302 1395 1347 1393 -321 2 -153
                2096 CD1 TYR 302 2.421 12.439 41.413 1.000 11.29
ATOM
                                                 302 2.421

302 1385

1246

1659

-58 98 - 46

302 2.859

13.075

40.248

1.000 10.60

302 1055

1241

1732

-11 52 - 1

302 0.161

12.793

40.858

1.000 11.30

-145 105 -
ANISOU 2096 CD1 TYR
                                                                              1246 1659 -58 98 - 46
                2097 CE1 TYR
ANISOU 2097 CE1 TYR
                2098 CD2 TYR
ANISOU 2098 CD2 TYR 302 1304
                                                                                                1656
                                                                                                                   -145 105 - 26
ATOM 2099 CE2 TYR 302 0.573
ANISOU 2099 CE2 TYR 302 1013
                                                                               13.406 39.690 1.000 11.72
                                                                               1733
                                                                                                 1708
                                                                                                                   -288 -138 1 6 1
                2100 CZ TYR 302 1.907 13.551 39.375 1.000 10.35
ANISOU 2100 CZ
                                     TYR 302 1009 1214
                                                                                                 1709
                                                                                                                   -229 -50 -19
                                    TYR 302 2.284 14.153 38.202 1.000 11.82
TYR 302 1192 1532 1766 -8 102 1 0 4
TYR 302 0.654 9.349 44.196 1.000 12.45
ATOM
                 2101 OH
ANISOU 2101 OH
ATOM
                 2102 C
ANISOU 2102 C
                                      TYR 302 1517 1450 1765
                                                                                                                   -181 -202 2 1 7
ATOM
                 2103 0
                                      TYR 302 -0.375 9.230 44.878 1.000 13.55
ANISOU 2103 O
                                      TYR 302 1464 1925 1759 -339 -211 7
             2104 N VAL 303 1.868 8.967 44.542 1.000 12.06
U 2104 N VAL 303 1517 1653 1413 -135 -3 3 4 0
2105 CA VAL 303 2.309 8.430 45.820 1.000 11.88
ATOM
ANISOU 2104 N
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- 159 -ANISOU 2105 CA VAL 303 1434 1609 1471 -368 -197 2 ATOM 2106 CB VAL 303 2.755 6.967 45.736 1.000 14.57 ANISOU 2106 CB VAL 303 1395 1682 2459 -217 -918 3 ATOM 2107 CG1 VAL 303 3.131 6.462 47.132 1.000 17.33 ANISOU 2107 CG1 VAL 303 2644 1608 2331 -48 -1114 -368 -197 2 2 3 -217 -918 3 1 2 VAL 303 2644 1608 2331 -48 -1114 VAL 303 1.703 6.041 45.122 1.000 14.80 VAL 303 1876 1676 2069 -592 -639 3 VAL 303 3.467 9.328 46.303 1.000 13.88 VAL 303 870 1791 2613 75 -286 -375 -48 -1114 6 1 2108 CG2 VAL 303 1.703 ANISOU 2108 CG2 VAL 303 1876 -592 -639 3 2 2 2109 C ATOM ANISOU 2109 C ATOM 2110 O VAL 303 4.526 9.417 45.681 1.000 19.70 2110 O VAL 303 1064 2307 4114 -61 323 -2111 N ASN 304 3.271 10.046 47.393 1.000 13.77 ANISOU 2110 O 323 - 999 MOTA ANISOU 2111 N ASN ATOM 2112 CA ASN ANISOU 2112 CA ASN ATOM 2113 CB ASN 304 1681 1815 1737 -479 -388 1 4 0 304 4.205 11.077 47.828 1.000 13.37 ANISOU 2112 CA ASN 304 1.205 11.077 47.828 1.000 13.37 ANISOU 2112 CA ASN 304 1626 1240 2212 -213 -533 2 ATOM 2113 CB ASN 304 3.460 12.223 48.566 1.000 13.24 ANISOU 2113 CB ASN 304 1206 1454 2370 -243 -344 2 ATOM 2114 CG ASN 304 2.457 ANISOU 2114 CG ASN 304 2142 2326 1910 146 -88 2 -213 -533 2 7 9 1454 2370 -243 -344 2 9 6 12.922 47.667 1.000 14.16 2114 CG ASN 304 1142 2326 1910 146 -88 2 3 0 2115 OD1 ASN 304 2.776 13.283 46.540 1.000 16.65 2115 OD1 ASN 304 1408 2456 2464 107 185 9 1 6 ANISOU 2115 OD1 ASN 304 1408 2115 OD1 ASN 304 1408 2456 2464 107 185 9 2116 ND2 ASN 304 1.263 13.126 48.209 1.000 17.45 2116 ND2 ASN 304 1414 2961 2257 545 181 3 ATOM ANISOU 2116 ND2 ASN 304 1414 545 181 315 ATOM. 2117 C ASN 304 5.325 10.588 48.728 1.000 11.18 ANISOU 2117 C ASN 304 1382 1299 1566 -183 -163 1 1 2 ATOM 2118 0 ASN 304 6.396 11.232 48.699 1.000 12.07 304 1325 1382 1879 -167 -66 - 9 305 5.092 9.541 49.516 1.000 12.56 305 1791 1296 1685 -152 -232 2 305 6.063 9.011 50.463 1.000 14.01 ANISOU 2118 O ASN -167 -66 -59 2119 N ATOM ILE ANISOU 2119 N ILE -152 -232 2 0 2 ATOM 2120 CA ILE ANISOU 2120 CA ILE -55 -479 7 9 9.493 51.906 1.000 14.44 2121 CB ILE 305 5.781 ANISOU 2121 CB ILE 305 2223 1604 1659 -29 -217 1 5 7 11.017 51.956 1.000 15.31 1608 2441 43 -479 - 31 ATOM 2122 CG2 ILE 305 5.725 ANISOU 2122 CG2 ILE 305 1768 1608 43 - 479 - 314 2441 2123 CG1 ILE ATOM 305 4.543 8.853 52.498 1.000 14.83 305 1779 1694 2163 27 -307 -15 ANISOU 2123 CG1 ILE 27 - 307 - 153 ATOM 2127 N ARG 306 7.170 6.896 50.829 1.000 13.04
ANISOU 2127 N ARG 306 1618 1389 1946 -368 -598 2
ATOM 2128 CA ARG 306 7.340 5.435 50 860
ANISOU 2128 CA ARG 306 1352
ANISOU 2129 CB ARG ANISOU 2120 CB A -1491 381 9 2 -260 -586 2 3 1 1564 2597 -185 -1008 2 7 7 6.896 50.829 1.000 13.04 2127 N ARG 306 1618 1389 1946 -368 -598 3 8 3 2128 CA ARG 306 7.340 5.435 50.868 1.000 11.82 2128 CA ARG 306 1352 1366 1773 -375 -154 4 4 4 2129 CB ARG 306 8.111 4.965 49.640 1.000 15.28 2129 CB ARG 306 1976 1941 1886 -368 -19 1 1 1 2 130 CG ARG 306 8.203 3.472 49.395 1.000 17.16 2130 CG ARG 306 2566 1953 ANISOU 2129 CB ARG 306 1976 MOTA ANISOU 2130 CG ARG 306 2566 1953 2001 -68 -68 7 6 2131 CD ARG 306 8.344 3.075 47.937 1.000 19.51 MOTA ANISOU 2131 CD ARG 306 2921 2361 2130 -397 -396 -3 306 7.078 3.198 47.212 1.000 20.65 -397 -396 - 302 ATOM 2132 NE ARG ANISOU 2132 NE ARG 306 2693 2309 2844 -1056 -310 2 1 4 2133 CZ 306 6.948 306 2006 306 8.013 MOTA 3.186 45.893 1.000 17.11 ARG ANISOU 2133 CZ ARG 2225 2268 45 - 91 5 9 6 2134 NH1 ARG 3.065 45.083 1.000 21.58 ANISOU 2134 NH1 ARG 306 2405 2677 3116 -232 381 -669 306 5.734 306 2235 2135 NH2 ARG 3.301 1550 45.365 1.000 17.51 ANISOU 2135 NH2 ARG 2868 150 -484 - 162

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- 160 -
ATOM 2136 C ARG 306 8.035
ANISOU 2136 C ARG 306 2254
ATOM 2137 O ARG 306 9.006
                                        5.027
                                                  52.155 1.000 13.45
                                        1018
                                       5.682
1099
                                                  1837 -246 -481 9 8
                                                  52.556 1.000 12.15
                                                  1615 -18 -362 - 8 0
52.811 1 000
ANISOU 2137 O
                    ARG
                          306 1902
                          307 7.571
MOTA
         2138 N
                    ARG
                                          3.968
                                                   52.811 1.000 18.19
                          307 3073
ANISOU 2138 N
                                         1620
                    ARG
                                                   2218 -734 -938 7 9 2
                                                  53.989 1.000 19.20
         2139 CA
MOTA
                          307 8.197
                                        3.380
                   ARG
ANISOU 2139 CA
                    ARG
                          307 3053
                                         1963
                                                   2277 -675 -1236 6 4 3
ATOM
         2140 C
                          307 9.086 2.191 53.611 1.000 23.08
                     ARG
ANISOU 2140 C
                    ARG 307 4018
                                         1905
                                                   2847 -270 -1885 3 2 9
                    ARG 307 8.636 1.292 52.895 1.000 35.93
MOTA
         2141 0
                          307 6003
                          307 7.131 2.918 54.997 1.000 28.25
307 5557 3297 1882 1500
ANISOU 2141 O
                    ARG
                                                             38 - 3227 - 791
         2142 CB
MOTA
                    ARG
ANISOU 2142 CB
                    ARG
                                                             -1503 -277 5 0 9
ATOM
         2143 CG
                           307 6.032 3.921
                    ARG
                                                  55.275 1.000 33.39
                          307 4564
ANISOU 2143 CG
                    ARG
                                         4859
                                                   3261
                                                             -1613 731 208
                          307 5.022 3.523
         2144 CD
                    ARG
                                                  56.317 1.000 40.42
ANISOU 2144 CD
                          307 6335
                    ARG
                                          5701
                                                   3322
                                                             -1900 1263 9 7 1
         2145 NE
ATOM
                          307 5.605
                    ARG
                                          2.952
                                                   57.529 1.000 50.83
ANISOU 2145 NE
                    ARG
                          307 8119 7287
                                                   3908
                                                             -2786 105 1624
                          307 4.894 2.441 58.530 1.000 51.36
ATOM
         2146 CZ
                    ARG
ANISOU 2146 CZ
                    ARG
                         307 7424 8064
                                                  4025
                                                             -3650 -966 2451
         2147 NH1 ARG
MOTA
                          307 3.567 2.422 58.485 1.000 69.51

      307
      3.567
      2.422
      58.485
      1.000 69.51

      307
      7586
      10951
      7874
      -6970 -2008 3 2 4 5

      307
      5.489
      1.937
      59.600
      1.000 59.99

      307
      10714
      8150
      3930
      -5986 -3291 2 0 2 8

      308
      10.347
      2.147
      54.048
      1.000 22.92

      308
      2759
      2587
      3364
      -589
      -200 1 7 0

      308
      11.215
      1.009
      53.794
      1.000 24.47

      308
      3382
      2649
      3268
      -360
      52 1 5 0

      308
      10.602
      -0.252
      54.382
      1.000 31.10

      308
      5251
      2520
      4044
      -768
      16 2 7 9

ANISOU 2147 NH1 ARG
        2148 NH2 ARG
ATOM
ANISOU 2148 NH2 ARG
        2149 N
ATOM
                    THR
ANISOU 2149 N
                    THR
         2150 CA THR
MOTA
ANISOU 2150 CA
                   \mathtt{THR}
MOTA
        2151 C
                    THR
                    THR 308 5251 2520 4044 -768 16 279
THR 308 10.610 -1.292 53.718 1.000 31.44
THR 308 4573 2676 4696 -457 -1745 -40
ANISOU 2151 C
ATOM
        2152 0
ANISOU 2152 O
ATOM 2153 CB
ANISOU 2153 CB
                    THR
                          308 12.615 1.279 54.378 1.000 23.51
                    THR
                          308 3718
                                         2086 3131 413 -694 5 4 2
ATOM
        2154 OG1 THR
                          308 13.195 2.410 53.705 1.000 23.61
ANISOU 2154 OG1 THR
                          308 2711 2503 3754
                                                            153 437 - 9
        2155 CG2 THR
                           308 13.573 0.141 54.117 1.000 26.37
ANISOU 2155 CG2 THR
                           308 4427
                                         2796
                                                   2796
                                                            927 -329 - 18
ATOM
        2156 N
                    SER
                          309 10.066
                                         -0.156 55.596 1.000 28.39
ANISOU 2156 N
                          309 3759
309 9.488
                    SER
                                         2774
                                                  4252
                                                            -19
ATOM
      2157 CA
                                         -1.335 56.238 1.000 34.69
                   SER
ANISOU 2157 CA
                          309 6110
                   SER
                                         3146
                                                   3925
                                                            -1066 -1089 1626
                                         -1.737 55.724 1.000 41.41
3910 5383 -2171 -1170
MOTA
        2158 C
                    SER
                          309 8.109
ANISOU 2158 C
                    SER
                         309 6442
                                                             -2171 -1170 2144
ATOM
        2159 0
                                         -2.884 55.952 1.000 57.05
5141 5146 -4907 -2077
                    SER 309 7.672
ANISOU 2159 O
ATOM 2160 CB
                    SER 309 11389
                                                            -4907 -2077 2027
                    SER
                          309 9.450
                                         -1.104 57.755 1.000 31.61
ANISOU 2160 CB
                          309 4863
                    SER
                                        2958
                                                   4188
                                                            -483 368 962
                          309 8.485
ATOM
        2161 OG
                    SER
                                        -0.135 58.107 1.000 38.99
                          309 4731
ANISOU 2161 OG
                    SER
                                        3477 6604
                                                          313 -2249 - 496
ATOM
        2162 N
                    LYS
                           310 7.391
                                         -0.868 55.032 1.000 47.69
                          310 5502
312 8.574
ANISOU 2162 N
                    LYS
                                         5577
                                                   7040
                                                            -539 -1369 1583
ATOM
        2163 FE
                    IUM
                                         13.466 54.055 1.000 11.05
ANISOU 2163 FE
                    IUM
                          312 1690
                                         1156 1351 -101 -237 7 1
MOTA
        2164 C1
                          313 5.987
313 2777
                    AKG
                                         14.815 54.612 1.000 19.65
ANISOU 2164 C1
                    AKG
                                         2119
                                                   2572 258 -117 5 5 6
ATOM
        2165 01
                    AKG
                          313 4.799
                                         15.240 54.659 1.000 20.82
ANISOU 2165 01
                          313 2957 2293 2659 514 -234 2 6 4
313 6.643 14.144 53.787 1.000 17.79
                          313 2957 2293
                    AKG
        2166 02
                    AKG
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- 161 -ANISOU 2166 02 AKG 313 2407 1765 2587 74 - 377 429 2167 C2 313 6.867 MOTA AKG 15.178 55.844 1.000 20.08 313 1997 313 7.982 313 2289 ANISOU 2167 C2 AKG 2566 3068 -528 419 -399 ATOM 2168 05 AKG 14.661 55.821 1.000 17.60 ANISOU 2168 05 AKG 2066 2334 -314 226 -252 ATOM 2169 C3 AKG 313 6.272 16.080 56.872 1.000 21.69 ANISOU 2169 C3 AKG 313 2751 1910 3581 240 62 - 327 2170 C4 ATOM AKG 313 7.318 16.741 57.716 1.000 21.50 ANISOU 2170 C4 AKG 313 3246 1761 199 3160 -143 - 185 2171 C5 ATOM AKG 313 6.923 17.816 58.672 1.000 22.58 ANISOU 2171 C5 AKG 313 3122 1840 3618 755 -495 - 313ATOM - 2172 03 AKG 313 7.754 18.591 59.124 1.000 27.48 ANISOU 2172 03 AKG 313 3581 2470 4389 -34 602 - 1266 ATOM 2173 04 AKG 313 5.660 17.889 58.999 1.000 28.55 ANISOU 2173 04 AKG 313 3191 2809 4846 612 -246 -1148 2174 S MOTA SO4 401 11.676 0.439 24.942 1.000 40.14 ATOM 2175 01 SO4 401 11.293 0.826 26.321 1.000 33.12 2176 02 ATOM SO4 401 12.501 -0.829 25.014 1.000 35.79 2177 03 ATOM 401 10.430 SO4 0.189 24.129 1.000 54.89 401 12.500 1.520 24.329 1.000 44.80 501 -6.455 10.219 44.319 1.000 14.29 502 -10.520 18.612 50.560 1.000 12.86 503 -8.644 16.907 47.858 1.000 16.83 504 -10.313 20.800 43.074 1.000 16.10 505 -6.051 19.199 52.602 1.000 16.38 2178 04 ATOM SO4 2179 OW MOTA НОН ATOM 2180 OW HOH 2181 OW ATOM HOH MOTA 2182 OW HOH 2183 OW ATOM HOH ATOM 2184 OW HOH 506 -6.873 24.642 47.100 1.000 20.55 ATOM 2185 OW HOH 507 10.676 -4.179 46.406 1.000 27.41 MOTA 2186 OW HOH 508 -0.077 21.786 40.872 1.000 15.22 2187 OW 509 5.761 ATOM HOH 13.656 46.041 1.000 17.40 ATOM 2188 OW 510 29.135 511 26.032 HOH 31.449 51.982 1.000 18.40 2189 OW ATOM 32.724 52.741 1.000 17.03 32.371 46.000 1.000 16.70 HOH 2190 OW ATOM HOH 512 10.965 513 23.871 514 26.353 24.457 58.649 1.000 18.71 29.063 50.326 1.000 18.96 33.106 53.153 1.000 20.41 11.721 55.329 1.000 18.39 15.567 53.585 1.000 24.87 ATOM HOH 2191 OW ATOM 2192 OW HOH 2193 OW ATOM HOH 515 23.191 2194 OW ATOM HOH 516 21.429 ATOM 2195 OW HOH 517 9.122 2196 OW MOTA HOH 518 27.843 17.352 53.437 1.000 27.76 ATOM 2197 OW HOH519 -14.415 20.029 44.444 1.000 23.47 ATOM 2198 OW HOH 520 15.253 33.050 51.771 1.000 27.20 ATOM 2199 OW 521 14.080 HOH 31.486 44.302 1.000 21.58 2200 OW ATOM HOH 522 17.770 33.842 53.596 1.000 23.56 ATOM 2201 OW HOH 523 3.671 24.673 36.173 1.000 20.95 ATOM 2202 OW НОН 524 -15.683 28.618 52.535 1.000 24.05 524 - 15.683 28.618 52.535 1.000 24.05 525 - 5.386 20.413 39.013 1.000 26.85 526 10.417 27.949 58.778 1.000 28.33 527 23.165 19.592 62.202 1.000 29.36 528 23.736 10.550 55.737 1.000 24.02 529 - 1.662 28.650 42.485 1.000 21.62 530 - 4.689 10.177 46.511 1.000 31.65 531 1.545 35.657 50.866 1.000 19.59 1.545 ATOM 2203 OW HOH ATOM 2204 OW HOH ATOM 2205 OW нон ATOM 2206 OW HOH ATOM 2207 OW нон ATOM 2208 OW HOHATOM 2209 OW HOH ATOM 2210 OW HOH 532 0.980 22.687 36.818 1.000 30.57 ATOM 2211 OW HOH 533 -12.450 16.848 56.071 1.000 28.42 ATOM 2212 OW HOH 534 -9.418 16.139 51.364 1.000 22.60 MOTA 2213 OW HOH 535 32.711 25.816 43.116 1.000 31.44 ATOM 2214 OW НОН 536 27.068 24.587 55.468 1.000 23.32 ATOM 2215 OW HOH 537 13.523 11.832 51.199 1.000 10.73 ATOM 2216 OW HOH 538 8.513 16.158 35.074 1.000 12.26 2217 OW ATOM HOH 539 0.922 2.590 35.058 1.000 14.79 2218 OW ATOM 540 -1.548 3.709 34.484 1.000 14.25 541 11.711 16.898 30.416 1.000 17.84 HOH MOTA 2219 OW HOH

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ATOM 2220 OW HOH 542 15.389 11.536 32.065 1.000 17.88 ATOM 2221 OW HOH 543 18.496 6.995 52.191 1.000 17.47 ATOM 2222 OW HOH 544 19.848 22.580 35.334 1.000 17.28 ATOM 2223 OW 545 -0.387 HOH 41.967 1.000 13.22 4.787 ATOM 2224 OW нон 546 23.502 12.662 35.308 1.000 18.14 ATOM 2225 OW нон 547 10.332 25.236 33.926 1.000 19.05 2226 OW MOTA нон 548 21.447 20.605 34.090 1.000 17.24 2227 OW ATOM HOH 549 8.164 7.685 27.077 1.000 25.40 ATOM 2228 OW HOH -5.127 40.321 1.000 15.88 550 14.393 29.356 39.662 1.000 16.45 24.144 58.426 1.000 19.71 7.949 33.182 1.000 17.90 2.691 43.340 1.000 23.76 28.057 40.079 1.000 18.44 ATOM 2229 OW нон 551 12.873 2230 OW ATOM HOH 552 11.974 ATOM 2231 OW HOH 553 17.521 MOTA 2232 OW нон 554 3.401 2233 OW ATOM HOH 555 18.669 2234 OW 12.928 30.017 1.000 19.57 ATOM HOH 556 10.827 ATOM 2235 OW 557 20.630 16.270 65.466 1.000 20.84 HOH ATOM 2236 OW 558 11.315 20.266 64.044 1.000 21.62 HOH ATOM 2237 OW 559 26.277 14.516 43.946 1.000 16.22 HOH ATOM 2238 OW 560 9.616 15.488 32.365 1.000 19.40 HOH 2239 OW MOTA HOH 561 8.888 4.903 27.857 1.000 22.74 2240 OW ATOM -1.851 42.511 1.000 22.98 29.415 38.332 1.000 26.36 HOH 562 20.496 ATOM 2241 OW 563 17.033 НОН 564 18.595 6.141 37.697 1.000 25.10 565 22.446 13.893 31.420 1.000 29.00 566 6.586 3.577 28.350 1.000 27.82 567 6.250 20.077 30.961 1.000 23.27 ATOM 2242 OW HOH ATOM 2243 OW HOH ATOM 2244 OW HOH 2245 OW ATOM HOH 567 6.250 20.077 30.961 1.000 23.27 2246 OW ATOM HOH 568 7.341 1.000 28.59 16.113 31.186 MOTA 2247 OW HOH 569 16.090 32.070 42.552 1.000 33.08 MOTA 2248 OW 570 11.500 28.806 37.258 1.000 25.17 HOHATOM 2249 OW HOH 571 12.901 26.768 58.591 1.000 28.58  $\mathtt{ATOM}$ 2250 OW HOH 572 -17.071 17.043 50.450 1.000 28.82 ATOM 2251 OW HOH 573 25.262 7.705 37.199 1.000 39.05 26.440 51.734 -1.000 29.03 19.088 42.527 1.000 14.86 ATOM 2252 OW HOH 574 32.884 2253 OW MOTA 575 -1.199 576 -4.389 HOH576 -4.389 33.026 63.392 1.000 29.56 577 17.569 25.732 32.249 1.000 20.62 578 -19.107 12.822 67.516 1.000 22.35 579 29.333 19.198 51.975 1.000 22.51 580 27.950 27.635 51.903 1.000 25.40 581 -21.085 14.501 68.535 1.000 21.19 MOTA 2254 OW HOH MOTA 2255 OW HOH ATOM 2256 OW HOH ATOM 2257 OW HOH MOTA 2258 OW HOH 2259 OW ATOM HOH ATOM 2260 OW HOH582 1.529 17.378 33.953 1.000 25.29 ATOM 2261 OW HOH 583 9.138 20.887 66.894 1.000 33.92 584 -11.896 19.091 44.780 1.000 17.48 585 6.382 12.597 43.347 1.000 22.09 MOTA 2262 OW HOH ATOM 2263 OW HOH ATOM 2264 OW HOH 586 17.762 21.268 29.046 1.000 20.79 ATOM 2265 OW 587 -11.500 25.438 41.729 1.000 29.68 HOH ATOM 2266 OW 588 7.877 HOH 1.046 29.689 1.000 27.70 589 27.985 13.540 42.235 1.000 25.91 2267 OW ATOM HOH MOTA 2268 OW 14.852 34.021 1.000 20.41 24.179 41.242 1.000 26.77 14.096 36.006 1.000 27.92 36.981 57.827 1.000 31.86 нон 590 1.276 ATOM 2269 OW HOH 591 24.622 ATOM 2270 OW HOH 592 0.404 ATOM 2271 OW 593 -2.835 HOH 2272 OW ATOM HOH 594 3.276 39.940 1.000 32.07 0.788 ATOM 2273 OW HOH 595 11.025 -8.794 31.468 1.000 27.18 2274 OW ATOM нон 596 6.301 2.276 42.639 1.000 29.74 MOTA 2275 OW HOH 597 29.302 16.146 62.924 1.000 43.75 2276 OW 2277 OW ATOM 598 19.039 HOH 20.964 67.011 1.000 30.85 MOTA HOH 599 8.380 22.088 64.518 1.000 42.62 ATOM 2278 OW нон 600 21.480 10.826 34.742 1.000 25.74 ATOM 2279 OW HOH 601 -2.907 21.956 38.566 1.000 30.92 2280 OW ATOM 602 -3.928 29.841 43.352 1.000 43.96 HOH

- 163 -ATOM 2281 OW HOH 603 2.885 21.563 34.437 1.000 33.10 MOTA 2282 OW 604 11.801 6.043 HOH 25.270 1.000 38.18 ATOM 2283 OW HOH 605 -1.019 17.197 40.472 1.000 18.48 2284 OW ATOM HOH 606 18.382 23.349 68.110 1.000 22.54 ATOM 2285 OW HOH 607 -8.141 8.137 45.609 1.000 17.64 ATOM 2286 OW HOH 608 5.022 2.667 51.700 1.000 24.29 MOTA 2287 OW HOH 609 17.557 10.755 33.490 1.000 21.94 ATOM 2288 OW нон 610 11.222 1.201 49.675 1.000 20.61 ATOM 2289 OW HOH 611 4.243 35.047 50.509 1.000 22.18 ATOM 2290 OW HOH 612 11.103 4.031 56.082 1.000 22.08 ATOM 2291 OW HOH 36.791 1.000 32.32 52.739 1.000 31.83 30.674 1.000 24.77 31.445 1.000 25.97 613 11.366 31.522 ATOM 2292 OW HOH 614 -21.189 24.787 ATOM 2293 OW НОН 615 7.847 -1.491 MOTA 2294 OW НОН 616 19.041 11.937 MOTA 2295 OW НОН 617 6.221 29.879 40.410 1.000 29.24 MOTA 2296 OW HOH 618 17.266 5.933 35.280 1.000 23.72 ATOM 2297 OW HOH 619 5.983 -7.215 28.510 1.000 28.19  $\mathtt{ATOM}$ 2298 OW HOH 620 22.574 8.129 57.639 1.000 30.97 ATOM 2299 OW НОН 621 2.553 7.806 60.287 1.000 28.77 2300 OW 

 622
 29.939
 25.812
 51.234
 1.000 34.00

 623
 2.205
 34.823
 53.632
 1.000 25.88

 ATOM HOH ATOM 2301 OW HOH ATOM 2302 OW 624 18.091 13.838 67.343 1.000 28.46 нон ATOM 2303 OW HOH 625 8.342 3.195 58.475 1.000 26.84 626 -16.086 18.427 42.790 1.000 31.11 627 -2.098 13.445 35.620 1.000 27.48 625 8.342 ATOM 2304 OW нон ATOM 2305 OW HOH 2306 OW ATOM HOH 628 0.481 30.471 42.834 1.000 32.55 ATOM 2307 OW HOH 629 13.368 33.845 42.899 1.000 28.70 2308 OW ATOM HOH 630 -13.792 14.642 51.533 1.000 25.58 ATOM 2309 OW HOH 631~3.299 29.242 1.000 39.62 1.461 MOTA 2310 OW нон 632 -16.012 20.690 46.705 1.000 27.75 ATOM 2311 OW HOH 633 19.606 8.142 31.259 1.000 27.02 ATOM 2312 OW HOH 634 5.077 7.954 57.205 1.000 30.59 2313 OW ATOM HOH 635 -1.502 6.963 45.877 1.000 35.68 636 9.974 17.449 38.804 1.000 21.84 637 -22.829 12.836 67.228 1.000 25.04 ATOM 2314 OW HOH ATOM 2315 OW HOH 638 6.275 34.333 39.722 1.000 25.88 639 2.248 19.798 56.051 1.000 26.67 640 -20.552 17.013 67.454 1.000 31.34 641 9.298 16.570 28.911 1.000 29.96 642 -1 732 11.113 60.074 1.000 28.13 MOTA 2316 OW НОН ATOM 2317 OW HOH 2318 OW ATOM HOH ATOM 2319 OW HOH 2320 OW ATOM HOH 11.113 60.074 1.000 28.13 ATOM 2321 OW HOH 643 34.157 44.657 1.000 36.36 23.604 ATOM 2322 OW HOH 644 24.298 33.576 1.000 34.90 20.199 ATOM 2323 OW 645 13.803 HOH 31.570 1.000 32.66 -4.667 MOTA 2324 OW HOH 646 6.295 -2.594 29.009 1.000 34.61 MOTA 2325 OW НОН 647 5.623 37.039 49.318 1.000 28.08 ATOM 2326 OW HOH 648 -18.805 19.286 46.868 1.000 38.32 2327 OW ATOM 649 16.026 35.829 49.382 1.000 34.45 HOH ATOM 2328 OW 650 -12.187 28.769 45.330 1.000 27.36 651 21.344 5.778 55.101 1.000 27.43 нон ATOM 2329 OW нон 5.778 55.101 1.000 27.43 
 652
 -1.848
 2.125
 32.240
 1.000
 27.43

 653
 -14.568
 18.811
 55.775
 1.000
 29.95

 654
 -8.655
 26.254
 38.301
 1.000
 32.07

 655
 18.836
 13.542
 28.102
 1.000
 32.07
 MOTA 2330 OW нон ATOM 2331 OW HOH ATOM 2332 OW нон 2333 OW ATOM нон 28.102 1.000 32.24 ATOM 2334 OW HOH 656 16.217 14.669 25.619 1.000 33.35 ATOM 2335 OW нон 657 28:678 14.477 38.043 1.000 30.94 2336 OW ATOM НОН 658 -11.834 15.408 53.330 1.000 33.25 ATOM 2337 OW нон 659 -1.317 38.273 59.599 1.000 34.45 ATOM 2338 OW HOH 660 8.784 28.681 1.000 33.62 13.918 ATOM 2339 OW HOH 661 -3.058 14.508 47.405 1.000 28.79 ATOM 2340 OW нон 662 10.968 33.651 38.533 1.000 36.21 ATOM 2341 OW HOH 663 28.960 21.602 53.665 1.000 29.25

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ATOM ATOM	2342 2343	WO WO	HOH HOH	664 665	-10.709 17.790	26.808	39.175 55.023	1.000 42.71
ATOM	2344	OW	HOH	666	6.404	24.865	29.848	1.000 34.55
ATOM	2345	OW	нон	667	-15.418	19.777	58.341	1.000 3 3 . 8 2
ATOM	2346	OW	HOH	668	0.000	0.000	37.259	0.330 49.90
ATOM	2347	OW	нон	669	19.652	24.610	33.660	1.000 31.77
ATOM	2348	OW	HOH	670	17.188	9.619	29.950	1.000 29.94
ATOM	2349	ow	HOH	671	17.708	2.958	28.338	1.000 29.94
ATOM	2350	OW	HOH	672	-0.059	3.652	30.079	1.000 3 2.23
MOTA	2351	OW	нон	673	29.037	20.923	56.153	1.000 28.52
ATOM	2352	ow	HOH	674	-15.435	31.088	53.795	1.000 35.61
MOTA	2353	OW	нон	675	-12.846		61.856	1.000 38.79
MOTA	2354	OW	HOH	676	10.299	39.666	49.554	1.000 40.30
MOTA	2355	ΟW	нон	677	-5.921	28.822	41.521	1.000 34.01
$\mathtt{MOTA}$	2356	ΟW	нон	678	6.029	39.991	46.094	1.000 42.69
ATOM	2357	WO	HOH	679	35.052	23.156	52.356	1.000 40.17
ATOM	2358	ΟW	$H \cup H$	680	-12.008	38.355	51.601	1.000 35.18
ATOM	2359	OM	HOH	681	3.061	13.047	53.152	1.000 35.17
ATOM	2360	OW	HOH	682	1.379	2.075	27.532	1.000 46.38
ATOM	2361	OW	HOH	683	-0.516	-2.480	37.686	1.000 21.77
ATOM	2362	OW	HOH	684	4.567	10.310	43.503	1.000 24.86
MOTA	2363	ΟW	HOH	685	19.443	5.558	61.133	1.000 36.06
MOTA	2364	OM	HOH	686	3.205	29.499	40.656	1.000 36.99
MOTA	2365	OW	нон	687	32.498	16.774	43.447	1.000 41.18
ATOM	2366	OW	НОН	688	28.166	23.113	57.593	1.000 35.56
ATOM	2367	OW	HOH	689	-17.023	23.220	46.759	1.000 30.05
ATOM	2368	OW	HOH	690	15.567	7.782	28.910	1.000 32.51
ATOM	2369	OW	HOH	691	11.780	30.287	57.203	1.000 33.34
ATOM	2370	OW	HOH	692	24.449	12.699	32.400	1.000 34.99
ATOM	2371	OW	нон	693	26.200	25.005	57.918	1.000 39.38

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#### **CLAIMS**

- 1. Deacetoxycephalosporin C synthase (DAOCS) having a structure designated by the X-ray co-ordinates of structure A or structure B herein.
- 2. DAOCS in the form of a complex with a metal, e.g. iron or lead, and optionally in the presence of a substrate and/or a substrate analogue or inhibitor, having a structure designated by the X-ray co-ordinates herein.
- 3. DAOCS as claimed in claim 2, wherein the substrate is penicillin N, penicillin G, 2-oxoglutarate or dioxygen, and the inhibitor is selected from N-oxalylamino acids, pyridine-carboxylates and nitrous oxide.
- 4. Use of the three-dimensional structure of DAOCS for the modification of DAOCS or other related 2-oxoglutarate dependent enzyme.
  - 5. Use as claimed in claim 4, wherein the related 2-oxoglutarate dependent enzyme is DACS, DAOC/DACS or the oxygenase enzyme involved in the introduction of the  $7\alpha$ -methoxy group into cephamycin C.
  - 6. Use as claimed in claim 5 for the modification of DAOCS, DACS or DAOC/DACS such that they accept unnatural substrates more efficiently than the wild type enzymes.

7. Use as claimed in claim 5 for the modification of DAOCS, DACS, DAOC/DACS such that they convert natural substrates to pharmaceuticals or useful intermediates in the preparation of pharmaceuticals.

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8. Use as claimed in claim 6 wherein the unnatural substrates are penicillins including penicillin G, penicillin V, 6-aminopenicillanic acid, amoxycillin, or penicillins with a phenyl glycine or p-hydroxyphenyl glycine side chain.

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- 9. Use as claimed in claim 6 wherein the unnatural substrate is a cephalosporin.
- 10. Use as claimed in claim 6 wherein the unnatural substrate is an amino acid, including the proteinogenic amino acids, or a peptide.
  - 11. Use as claimed in any one of claims 6-8, wherein penicillin G, penicillin V, another unnatural substrate or penicillin N is converted to a cephalosporin or exomethylene cephalosporin.

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- An enzyme having significant (as herein defined) sequence similarity to DAOCS wherein the side chain binding site of penicillin N or DAOC is modified and at at least one of the following sites at least one amino acid residue is changed to another amino acid residue or is deleted: Thr72, Arg74, Arg75, Glu156, Leu158, Arg160, Arg162, Leu186, Ser187,
- Thr72, Arg74, Arg75, Glu156, Leu158, Arg160, Arg162, Leu186, Ser187, Phe225, Phe264, Arg266, Asp301, Tyr302, Val303, Asn304; and/or at least one additional amino acid residue is inserted within the region 300-311; provided that other residues interacting with the above may be changed in order to accommodate the change in one of the above.

13. An enzyme having significant (as herein defined) sequence similarity to DAOCS wherein the penicillin/cephalosporin binding site of penicillin N or DAOC is modified and at at least one of the following amino acid residues is changed or deleted: Ile88, Arg160, Arg162, Phe164, Met180, Thr190, Ile192, Phe225, Pro241, Val245, Val262, Phe264, Ile305, Arg306, Arg307; and/or at least one additional amino acid residue is inserted within the region 300-311; provided that other residues interacting with the above may be changed in order to accommodate the change in one of the above.

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- 14. An enzyme according to claim 12 or claim 13 which is a mutant of DAOCS or DACS or DAOC/DACS.
- 15. An enzyme as claimed in any one of claims 12-14, wherein both the side chain and the penicillin/cephalosporin binding sites of penicillin N or DAOC are modified and at least one of the residues specified in claims 12 and 13 is changed or deleted.
- 16. An enzyme as claimed in any one of claims 12-15, wherein
  two or more complementary mutations are introduced to create or delete a
  binding interaction, including H-bonds, electrostatic, or hydrophobic
  interactions
  - 17. A gene encoding for the enzyme of any one of claims 12-16.

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- 18. A micro-organism capable of expressing the gene of claim 17 under fermentation conditions.
- 19. Use of micro-organisms of claim 18 for the production of
   30 beta-lactams of the penicillin or cephalosporin (including cepham) families.

- 20. Use as claimed in claim 19 wherein the micro-organism contains another modified enzyme of the penicillin and cephalosporin biosynthesis pathway including isopenicillin N synthase, amidohydrolase/acetyltransferase, or L-delta-(aminoadipoyl)-L-cysteine-D-valine (ACV) synthetase.
- 21. A method which comprises using the three-dimensional structure of DAOCS for determining or predicting the structure of another related 2-oxoglutarate dependent enzyme or related enzyme not from the penicillin and cephalosporin biosynthesis pathway, and using the structural information so obtained for modifying the other enzyme or for designing an inhibitor for the other enzyme.
- 22. A method as claimed in claim 21 wherein the said other related 2-oxoglutarate dependent enzyme or related enzyme is 1-aminocylopropane-1-carboxylate oxidase, gibberellin C-20 oxidase, flavone synthase, flavanone 3β-hydroxylase, hyoscyamine 6β-hydroxylase, prolyl 4-hydroxylase, prolyl 3-hydroxylase, aspartyl hydroxylase, lysyl hydroxylase, proline hydroxylases, γ-butyrobetaine hydroxylase, enzymes in herbicide resistance mechanisms, clavaminate synthase, an oxygenase enzyme involved in the biosynthesis of carbapenems, the so called ethylene forming enzyme from *Pseudomonas syringe*, p-hydroxyphenylpyruvate dioxygenase, and an oxygenase enzyme involved in the oxidation of phytol in human liver peroxisomes.

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A method as claimed in claim 21 or 22, wherein the said other enzyme is modified, by deletion or addition or alteration; at one or more of the sites defined in claim 12 or claim 13; or using the following information for the design or an inhibitor: Asp185, His183 and His243 act as ligands to the iron; Arg258 and Ser260 and the Fe bind the

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2-oxoglutarate; Met180, Phe225, Leu31 and Val245 are close to the iron binding site; Tyr33, Arg160, Arg162, Phe164, Ile192, Gln194, Leu204, Leu223, Leu215 are important for the construction of the part of the active site binding 2-oxoglutarate; and Arg160 and Arg162 are important for binding an amino acid or peptide derived substrate.

- A method as claimed in any one of claims 21-23, wherein the said other enzyme is prolyl 4-hydroxylase, prolyl 3-hydroxylase, aspartyl hydroxylase, or lysyl hydroxylase and the inhibitor is to be used for the treatment of human diseases including fibrotic diseases including liver cirrhosis and arthritis.
- A method as claimed in any one of claims 21-23, wherein the said other enzyme is p-hydroxyphenylpyruvate dioxygenase and the inhibitor is to be used in the treatment of certain genetic disorders.
- A method as claimed in any one of claims 21-23, wherein the said other enzyme is involved in herbicide resistance and the information is to be used to design new herbicides to overcome the problem of resistance.

SUBSTITUTE SHEET (RULE 26)

# SUBSTITUTE SHEET (RULE 26)

## INTERNATIONAL SEARCH REPORT

Inte. .ional Application No

		PC1/GB 98	/ U3860			
A. CLASS IPC 6	SIFICATION OF SUBJECT MATTER C12N15/52 C12N9/00 C12P35	5/00	······································			
According t	to International Patent Classification (IPC) or to both national class	sification and IPC				
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Minimum d IPC 6	ocumer::ation searched (classification system followed by classifi C12N C12P	cation symbols)				
	tion searcned other than minimum documentation to the extent th					
Electronic	data base consulted during the international search (name of data	base and, where practical, search terms used				
C. DOCUM	ENTS CONSIDERED TO BE RELEVANT					
Category '	Citation of document, with indication, where appropriate, of the	relevant passages	Relevant to claim No.			
Х	CORTES, JESUS ET AL: "Purifica characterization of a	tion and	1			
V	2-oxoglutarate-linked ATP-independent deacetoxycephalosporin C synthase of Streptomyces lactamdurans"  J. GEN. MICROBIOL. (1987), 133(11), 3165-74 CODEN: JGMIAN; ISSN: 0022-1287, 1987, XP000035085					
Y	see the whole document	-/	2,3, 21-26			
X Furth	er documents are listed in the continuation of box C.	X Patent family members are listed in	n annex.			
"A" docume: conside	egories of cited documents:  Int defining the general state of the lart which is not ared to be of particular relevance ocument but published on or after the linternational at a second control of the c	"T" later document published after the interior priority date and not in conflict with tocited to understand the principle or the invention  "X" document of particular relevance; the cla	he application but ory underlying the			
"L" document which may throw doubts on priority claim(s) or which is cited to establish the publication date of another citation or other special reason (as specified)  "O" document referring to an oral disclosure, use, exhibition or other means "P" document published prior to the international filling date but  "Cument published prior to the international filling date but  "Cument published prior to the international filling date but  "Cument published prior to the international filling date but  "Cument published prior to the international filling date but  "Cument published prior to the international filling date but  "Cument published prior to the international filling date but  "Cument published prior to the international filling date but  "Cument be considered novel or cannot be considered to involve an inventive step when the document of particular relevance; the claimed inventive step when the document is combined with one or more other such document is combined with one or more other such document is combined with one or more other such document is combined with one or more other such document is combined with one or more other such document is combined with one or more other such document is combined with one or more other such document is combined with one or more other such document is combined with one or more other such document is combined with one or more other such document is combined with one or more other such document is combined with one or more other such document is cannot be considered novel or cannot be considered to involve an inventive step when the document is taken alone cannot be considered to involve an inventive and inven						
later tha	an the priority date claimed	"&" document member of the same patent fa	amily			
	ctual completion of the international search March 1999	Date of mailing of the international sear 26/03/1999	ch report			
Name and m	ailing address of the ISA European Patent Office, P.B. 5818 Patentiaan 2 NL - 2280 HV Rijswijk Tel. (-31-70) 340-2040, Tx. 31 651 epo nl, Fax: (+31-70) 340-3016	Authorized officer Hix, R				

### INTERNATIONAL SEARCH REPORT

Int. donal Application No PCT/GB 98/03860

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	ation) DOCUMENTS CONSIDERED TO BE RELEVANT	
Category -	Citation of document, with indication, where appropriate, of the relevant passages	Relevant to claim No.
X	ROLLINS, M. J. ET AL: "Purification and initial characterization of deacetoxycephalosporin C synthase from Streptomyces clavuligerus" CAN. J. MICROBIOL. (1988), 34(11), 1196-202 CODEN: CJMIAZ;ISSN: 0008-4166, 1988, XP002095821	1
Y	see the whole document	2,3, 21-26
X .	ROLLINS M J ET AL: "ISOPENICILLIN N SYNTHASE AND DEACETOXYCEPHALOSPORIN C SYNTHASE ACTIVITIES DURING DEFINED MEDIUM FERMENTATIONS OF STREPTOMYCES-CLAVULIGERUS EFFECT OF OXYGEN AND IRON SUPPLEMENTS" CAN J MICROBIOL, (1989) 35 (12), 1111-1117. CODEN: CJMIAZ. ISSN: 0008-4166., XP002095822	1
Y	see the whole document	2,3, 21-26
X	DOTZLAF, JOE E. ET AL: "Purification and properties of deacetoxycephalosporin C synthase from recombinant Escherichia coli and its comparison wit the native enzyme purified from Streptomyces clavuligerus" J. BIOL. CHEM. (1989), 264(17), 10219-27 CODEN: JBCHA3; ISSN: 0021-9258, 1989, XP002095823	1
(	see the whole document	2,3, 21-26
x	BALDWIN J E ET AL: "HIGH-LEVEL SOLUBLE EXPRESSION AND PURIFICATION OF DEACETOXYCEPHALOSPORIN C SYNTHASE." BIOORG MED CHEM LETT, (1992) 2 (7), 663-668. CODEN: BMCLE8. ISSN: 0960-894X., XP002095824	1
(	see the whole document	2,3, 21-26
(	EP 0 366 354 A (LILLY CO ELI) 2 May 1990 see the whole document	1 2,3, 21-26
(	BALDWIN J E ET AL: "HIGH-LEVEL SOLUBLE EXPRESSION AND PURIFICATION OF DEACETOXYCEPHALOSPORIN C SYNTHASE." BIOORG MED CHEM LETT, (1992) 2 (7), 663-668. CODEN: BMCLE8. ISSN: 0960-894X., XP002095825	1
<b>,</b>	see the whole document	2,3, 21-26
	-/	

#### IN RNATIONAL SEARCH REPORT

Inter onal Application No PCT/GB 98/03860

C.(Continu	ation) DOCUMENTS CONSIDERED TO BE RELEVANT	PCT/GB 98/03860
Category		Relevant to claim No.
P,X	VALEGARD, KARIN ET AL: "Structure of a cephalosporin synthase" NATURE (LONDON) (1998), 394(6695), 805-809 CODEN: NATUAS; ISSN: 0028-0836, 1998,	1-11, 21-26
P,X	XP002095826 see the whole document WO 98 16648 A (BALDWIN JACK EDWARD	1-26
	;CLIFTON IAN (GB); ISIS INNOVATION (GB); ROACH) 23 April 1998 see the whole document	
Y	ROACH P L ET AL: "CRYSTAL STRUCTURE OF ISOPENICILLIN N SYNTHASE IS THE FIRST FROM A NEW STRUCTURAL FAMILY OF ENZYMES" NATURE, vol. 375, no. 6533, 22 June 1995, pages 700-704, XP002059796 cited in the application see the whole document	2,3,21-26
Y	SCOTT R A ET AL: "X-RAY ABSORPTION SPECTROSCOPIC STUDIES OF THE HIGH-SPIN IRON(II) ACTIVE SITE OF ISOPENICILLIN N SYNTHASE: EVIDENCE FOR FE-S INTERACTION IN THE ENZYME-SUBSTRATE COMPLEX" BIOCHEMISTRY, vol. 31, no. 19, 1992, pages 4596-4601, XP002067783 see the whole document	2,3, 21-26
Y	ROACH P L ET AL: "STRUCTURE OF ISOPENICILLINN SYNTHASE COMPLEXED WITH SUBSTRATE AND THE MECHANISM OF PENICILLIN FORMATION" NATURE, vol. 387, no. 6635, 19 June 1997, pages 827-830, XP002067787 cited in the application see the whole document	2,3, 21-26
4	WO 97 20053 A (GIST BROCADES BV ;UNIV OXFORD (GB); SUTHERLAND JOHN DAVID (GB); BO) 5 June 1997 cited in the application see the whole document	
4	EP 0 532 341 A (MERCK & CO INC) 17 March 1993 cited in the application see the whole document	

## INTERNATIONAL SEARCH REPORT

Inte. .ional Application No PCT/GB 98/03860

		PC1/GB 9	57 03800
	ation) DOCUMENTS CONSIDERED TO BE RELEVANT		
Category '	Citation of document, with indication, where appropriate, of the relevant passages		Relevant to claim No.
A	N. SHIBATA ET AL.:  "Adipoyl-6-aminopenicillanic acid is a substrate for deacetoxycephalosporin C synthase (DAOCS)."  BIOORGANIC & MEDICINAL CHEMISTRY LETTERS, vol. 6, no. 113, 1996, pages 1579-1584, XP002095827 cited in the application see the whole document		
		_	
	, .		

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### INTERNATIONAL SEARCH REPORT

Information on patent family members

Inte ...onal Application No
PCT/GB 98/03860

r		FCI/GB	98/03860
Patent document cited in search report	Publication date	Patent family member(s)	Publication date
EP 0366354	A 02-05-1990	US 5082772 A DE 68925338 D DE 68925338 T DK 521489 A ES 2082787 T GR 3018596 T IL 92079 A JP 2242675 A	21-01-1992 15-02-1996 05-06-1996 25-04-1990 01-04-1996 30-04-1996 26-08-1994 27-09-1990
WO 9816648	A 23-04-1998	NONE	
WO 9720053	A 05-06-1997	AU 1097297 A EP 0863989 A GB 2323361 A	19-06-1997 16-09-1998 23-09-1998
EP 0532341	A 17-03-1993	US 5318896 A AT 173017 T AU 657787 B AU 2354292 A BG 98643 A CA 2077921 A,C CN 1075336 A CZ 9400532 A DE 69227494 D EP 0843013 A FI 941135 A HU 69801 A IL 103076 A JP 7501931 T KR 132440 B MX 9205175 A NO 940848 A NZ 244236 A PL 174984 B SK 28894 A WO 9305158 A	07-06-1994 15-11-1998 23-03-1995 18-03-1993 31-03-1995 12-03-1993 17-08-1994 10-12-1998 20-05-1998 10-03-1994 28-09-1995 31-10-1996 02-03-1995 14-04-1998 28-02-1994 10-03-1994 25-03-1994 30-10-1998 07-09-1994 18-03-1994